Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTANXR1625

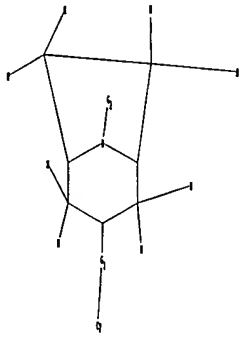
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

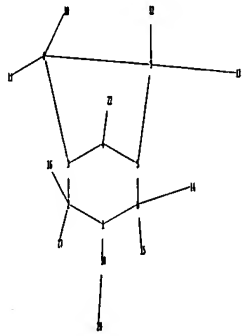
* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 5	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 7	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 8	JAN 29	PHAR reloaded with new search and display fields
NEWS 9	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 11	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 12	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13	FEB 26	MEDLINE reloaded with enhancements
NEWS 14	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 15	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 16	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 18	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19	MAR 16	CASREACT coverage extended
NEWS 20	MAR 20	MARPAT now updated daily
NEWS 21	MAR 22	LWPI reloaded
NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 23	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 24	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 26	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 28	MAY 01	New CAS web site launched
NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 30	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS EXPRESS		NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS LOGIN		Welcome Banner and News Items
NEWS IPC8		For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

```
* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:22:30 ON 15 MAY 2007

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:22:39 ON 15 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   14 MAY 2007  HIGHEST RN 934733-40-1
DICTIONARY FILE UPDATES:  14 MAY 2007  HIGHEST RN 934733-40-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10561417.str
```





chain nodes :
10 11 12 13 14 15 16 17 18 20 22
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
1-18 2-16 2-17 4-22 6-14 6-15 7-12 7-13 8-10 8-11 18-20
ring bonds :
1-2 1-6 2-3 3-4 3-8 4-5 5-6 5-7 7-8
exact/norm bonds :
1-2 1-6 1-18 2-3 3-4 4-5 4-22 5-6 18-20
exact bonds :
2-16 2-17 3-8 5-7 6-14 6-15 7-8 7-12 7-13 8-10 8-11
isolated ring systems :
containing 1 :

G1:O,S,N

G2:C,H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 20:Atom
22:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:23:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1296 TO ITERATE

100.0% PROCESSED 1296 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 23761 TO 28079
PROJECTED ANSWERS: 899 TO 1901

L2 50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 10:23:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 25160 TO ITERATE

100.0% PROCESSED 25160 ITERATIONS 1572 ANSWERS
SEARCH TIME: 00.00.01

L3 1572 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.55 172.76

FILE 'CAPLUS' ENTERED AT 10:23:34 ON 15 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 15 May 2007 VOL 146 ISS 21
FILE LAST UPDATED: 14 May 2007 (20070514/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3 full
L4 270 L3

=> s l4 and py<2003
22885312 PY<2003
L5 189 L4 AND PY<2003

=> d ibib abs hitstr 1-10

L5 ANSWER 1 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:978630 CAPLUS
DOCUMENT NUMBER: 138:39184
TITLE: Preparation of bridged bicyclic amino-substituted pyrrolidine modulators of CCR5 chemokine receptor activity
INVENTOR(S): Willoughby, Christopher A.; Rosauer, Keith; Chapman, Kevin T.; Mills, Sander G.; Shen, Dong-Ming; Shu, Min
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 46 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002198178	A1	20021226	US 2001-974643		20011010 <--
US 6531484	B2	20030311			
PRIORITY APPLN. INFO.:			US 2000-240598P	P	20001011
OTHER SOURCE(S):	MARPAT 138:39184				

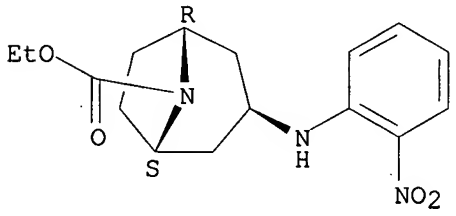
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = COOH, NO2, tetrazolyl, etc.; R2 = H, alkyl; Q = (CH2)3, CH2OCH2, CH2S1-2CH2, etc.; j, k, l, m, n = 0-3; R3, R5 = Ph, naphthyl, heterocycle; R4 = H, alkyl; R6 = H, alkyl, cycloalkyl, etc.; R7 = H, alkyl; R8a-8b = H, alkyl, alkenyl, alkynyl, cycloalkyl, Ph, etc.] are prepared For instance, reductive alkylation of tropine-derived benzimidazole II (preparation given) and a substituted homochiral pyrrolidine-aldehyde (preparation given; 1,2-dichloroethane, NaBH(OAc)3) produced III. I are modulators of CCR5 chemokine receptor activity and are useful, e.g., in the prevention or treatment of infection by HIV and the treatment of AIDS as ingredients in pharmaceutical compns., optionally in combination with other antivirals, immunomodulators, antibiotics or vaccines. Methods of treating AIDS and methods of preventing or treating infection by HIV are also described.
IT 208046-27-9P 280762-11-0P 280762-13-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bridged bicyclic amino substituted pyrrolidine modulators of CCR5 chemokine receptor activity)

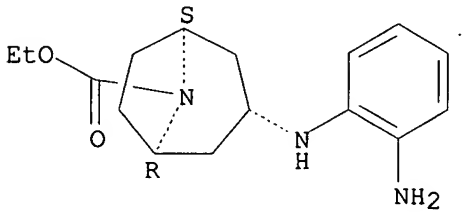
RN 208046-27-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-carboxylic acid, 3-[(2-nitrophenyl)amino]-, ethyl ester, (3-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



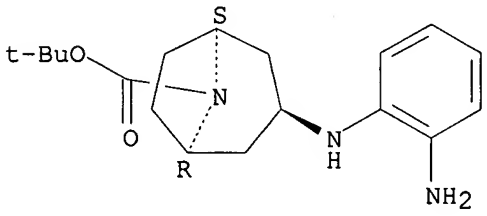
RN 280762-11-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-carboxylic acid, 3-[(2-aminophenyl)amino]-, ethyl ester, (3-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 280762-13-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-carboxylic acid, 3-[(2-aminophenyl)amino]-, 1,1-dimethylethyl ester, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



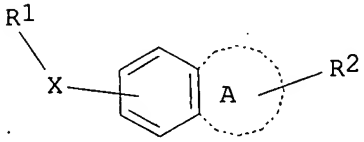
L5 ANSWER 2 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:964330 CAPLUS
DOCUMENT NUMBER: 138:39295
TITLE: Preparation of heterocyclic compounds as Rho-kinase inhibitors
INVENTOR(S): Imazaki, Naonori; Kitano, Masafumi; Ohashi, Naohito; Matsui, Kazuki
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Company, Limited, Japan
SOURCE: PCT Int. Appl., 425 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2002100833	A1	20021219	WO 2002-JP5609		20020606 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2002306284	A1	20021223	AU 2002-306284		20020606 <--
EP 1403255	A1	20040331	EP 2002-733352		20020606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
US 2004138286	A1	20040715	US 2003-480526		20031212
US 7199147	B2	20070403			
PRIORITY APPLN. INFO.:			JP 2001-176826	A	20010612
			JP 2001-398992	A	20011228
			WO 2002-JP5609	W	20020606

OTHER SOURCE(S): MARPAT 138:39295

GI



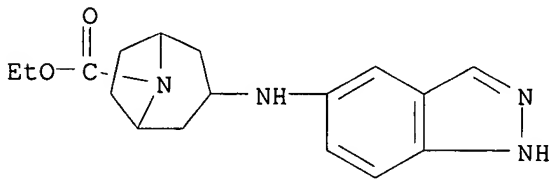
I

AB The title compds. I [wherein one to four groups represented by the general formula R1-X are present and may be the same or different from each other; A is a saturated or unsatd. five-membered heterocycle; X is a single bond, N(R3), O, S, or the like; R1 is hydrogen, halogeno, nitro, carboxyl, substituted or unsubstituted alkyl, or the like; R2 is hydrogen, halogeno, nitro, carboxyl, substituted or unsubstituted alkyl, or the like; and R3 is hydrogen, substituted or unsubstituted alkyl, or the like] are prepared N-(1-Benzyl-4-piperidinyl)-1H-indazole-5-amine dihydrochloride monohydrate in vitro showed IC50 of 0.4 μL/mL against Rho-kinase.

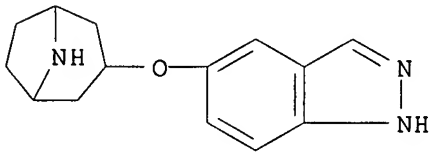
IT 478826-71-0P 478834-96-7P, 5-(8-Azabicyclo[3.2.1]oct-3-yloxy)-1H-indazole 478835-12-0P, N-(8-Benzyl-8-azabicyclo[3.2.1]oct-3-yl)-4-methyl-1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-amine 478835-16-4P, N-(8-Benzyl-8-azabicyclo[3.2.1]oct-3-yl)-4-methyl-1H-indazol-5-amine 478835-20-0P, N-(8-Azabicyclo[3.2.1]oct-3-yl)-4-methyl-1H-indazol-5-amine 478835-24-4P, N-(8-Propyl-8-azabicyclo[3.2.1]oct-3-yl)-4-methyl-1H-indazol-5-amine 478835-26-6P, 1-(Methylsulfonyl)-N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)-4-methyl-1H-indazol-5-amine 478835-29-9P, 3-Bromo-N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)-1H-indazol-5-amine 478835-32-4P, N-(1H-Indazol-5-yl)-N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)methanesulfonamide 478835-33-5P, N-(1H-Indazol-5-yl)-N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)acetamide 478835-89-1P, N-(8-Azabicyclo[3.2.1]oct-3-yl)-1H-indazol-5-amine 478836-33-8P, N-(8-Methyl-8-azabicyclo[3.2.1]oct-3-yl)-1H-indazol-5-amine 478836-54-3P, N-(8-(2-Phenoxyethyl)-8-azabicyclo[3.2.1]oct-3-yl)-1H-indazol-5-amine 478836-57-6P, N-(8-Propyl-8-azabicyclo[3.2.1]oct-3-yl)-1H-indazol-5-amine 478836-60-1P, N-(8-Isopropyl-8-azabicyclo[3.2.1]oct-3-yl)-1H-indazol-5-amine 478836-63-4P, N-(8-Isobutyl-8-azabicyclo[3.2.1]oct-3-yl)-1H-indazol-5-amine 478836-65-6P, N-[8-(Cyclobutylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]-1H-indazol-5-amine 478836-67-8P, N-[8-(Cyclohexylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]-1H-indazol-5-amine 478836-69-0P, N-[8-(2-Phenylethyl)-8-

azabicyclo[3.2.1]oct-3-yl]-1H-indazol-5-amine 478836-71-4P, 2-[3-(1H-Indazol-5-ylamino)-8-azabicyclo[3.2.1]oct-8-yl]ethanol 478836-73-6P, 2-[3-(1H-Indazol-5-ylamino)-8-azabicyclo[3.2.1]oct-8-yl]propan-1-ol 478836-75-8P, N-[8-(2-Methoxyethyl)-8-azabicyclo[3.2.1]oct-3-yl]-1H-indazol-5-amine 478836-77-0P, N-[8-(Tetrahydro-2H-pyran-2-ylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]-1H-indazol-5-amine 478836-79-2P, 2-[3-(1H-Indazol-5-ylamino)-8-azabicyclo[3.2.1]oct-8-yl]propanenitrile 478836-81-6P, 2-[3-(1H-Indazol-5-ylamino)-8-azabicyclo[3.2.1]oct-8-yl]acetamide 478837-69-3P 478837-71-7P 478837-73-9P 478837-75-1P 478837-77-3P 478837-79-5P 478837-82-0P 478837-84-2P 478837-86-4P 478837-90-0P 478838-01-6P 478838-04-9P 478838-06-1P 478838-10-7P 478838-12-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. as Rho-kinase inhibitors)

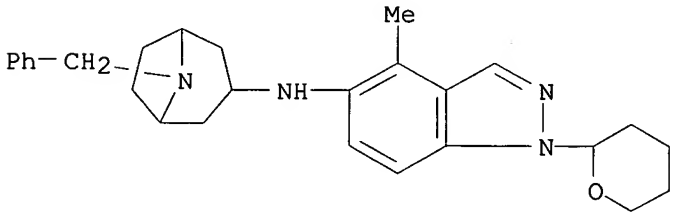
RN 478826-71-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-carboxylic acid, 3-(1H-indazol-5-ylamino)-, ethyl ester (9CI) (CA INDEX NAME)



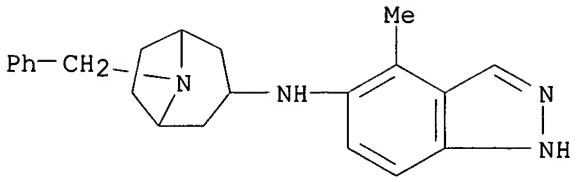
RN 478834-96-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane, 3-(1H-indazol-5-yloxy)- (9CI) (CA INDEX NAME)



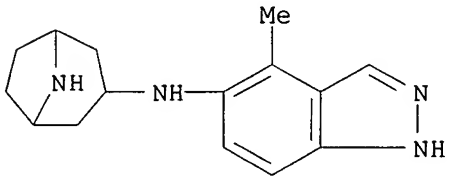
RN 478835-12-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-[4-methyl-1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-yl]-8-(phenylmethyl)- (9CI) (CA INDEX NAME)



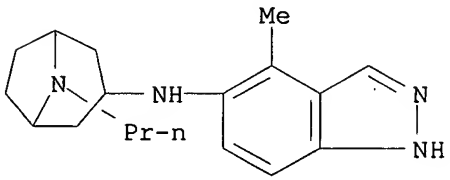
RN 478835-16-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-(4-methyl-1H-indazol-5-yl)-8-(phenylmethyl)- (9CI) (CA INDEX NAME)



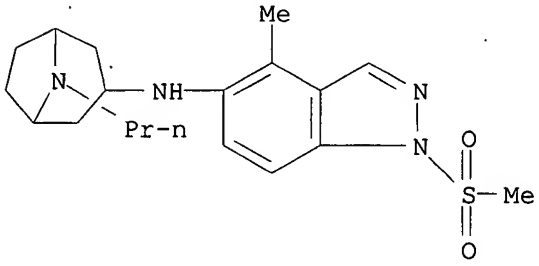
RN 478835-20-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-(4-methyl-1H-indazol-5-yl)- (9CI) (CA INDEX NAME)



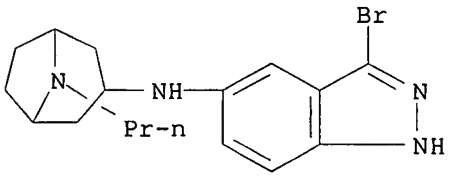
RN 478835-24-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-(4-methyl-1H-indazol-5-yl)-8-propyl- (9CI) (CA INDEX NAME)



RN 478835-26-6 CAPLUS
CN 1H-Indazol-5-amine, 4-methyl-1-(methylsulfonyl)-N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)- (9CI) (CA INDEX NAME)

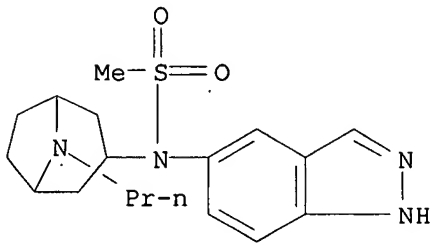


RN 478835-29-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-(3-bromo-1H-indazol-5-yl)-8-propyl- (9CI) (CA INDEX NAME)

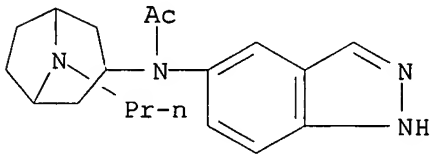


RN 478835-32-4 CAPLUS

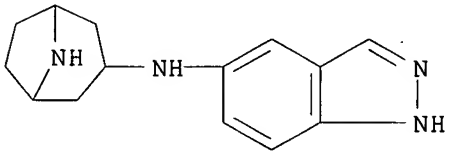
CN Methanesulfonamide, N-1H-indazol-5-yl-N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)- (9CI) (CA INDEX NAME)



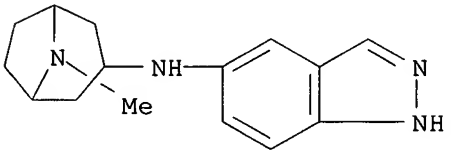
RN 478835-33-5 CAPLUS
CN Acetamide, N-1H-indazol-5-yl-N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)- (9CI) (CA INDEX NAME)



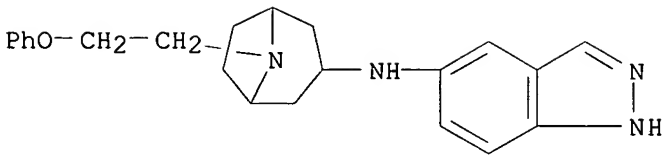
RN 478835-89-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



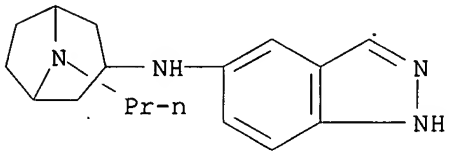
RN 478836-33-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-methyl- (9CI) (CA INDEX NAME)



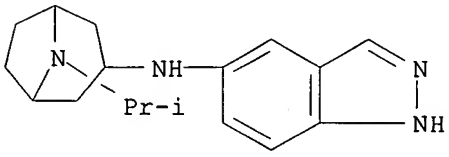
RN 478836-54-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(2-phenoxyethyl)- (9CI) (CA INDEX NAME)



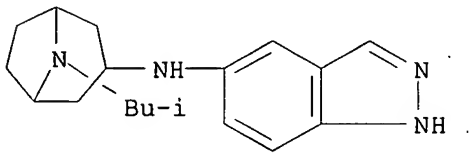
RN 478836-57-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-propyl- (9CI) (CA INDEX NAME)



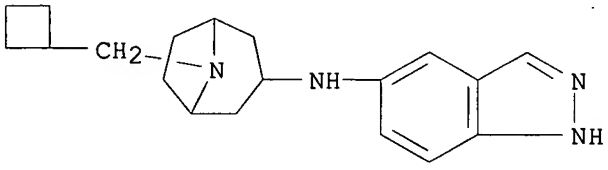
RN 478836-60-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



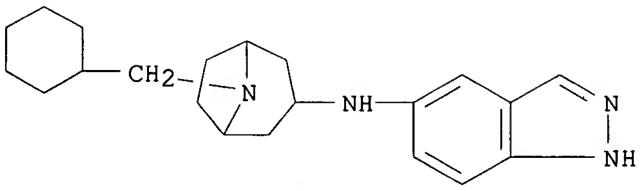
RN 478836-63-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(2-methylpropyl)- (9CI) (CA INDEX NAME)



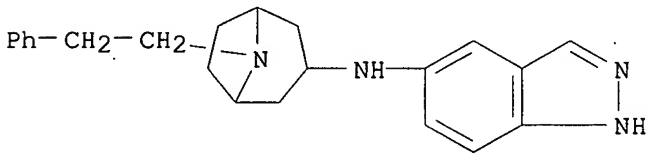
RN 478836-65-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-(cyclobutylmethyl)-N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



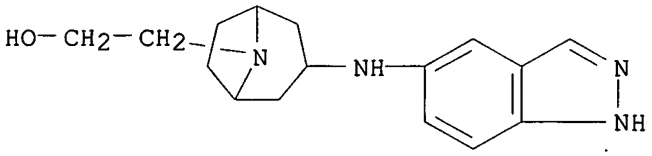
RN 478836-67-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-(cyclohexylmethyl)-N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



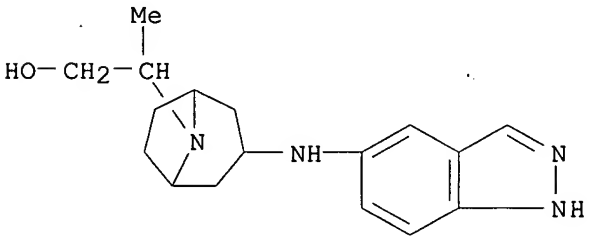
RN 478836-69-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(2-phenylethyl)- (9CI) (CA INDEX NAME)



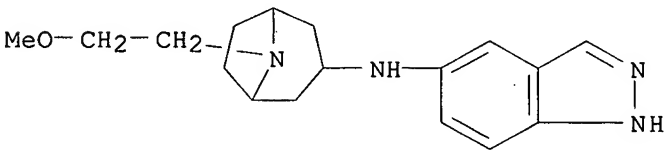
RN 478836-71-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-ethanol, 3-(1H-indazol-5-ylamino)- (9CI) (CA INDEX NAME)



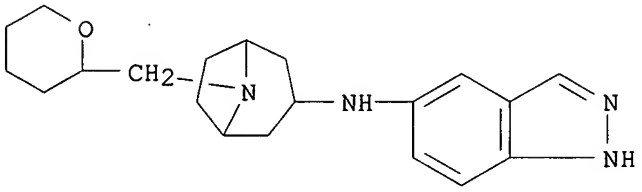
RN 478836-73-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-ethanol, 3-(1H-indazol-5-ylamino)-β-methyl- (9CI) (CA INDEX NAME)



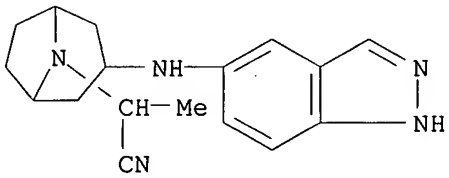
RN 478836-75-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



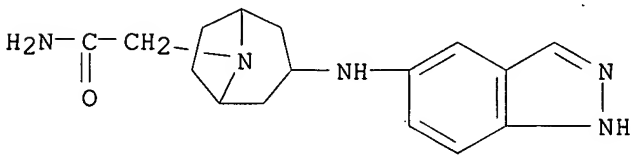
RN 478836-77-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-[(tetrahydro-2H-pyran-2-yl)methyl]- (9CI) (CA INDEX NAME)



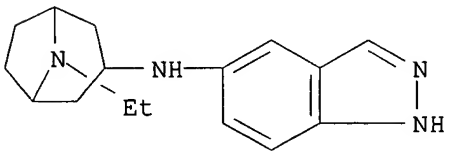
RN 478836-79-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-acetonitrile, 3-(1H-indazol-5-ylamino)-α-methyl- (9CI) (CA INDEX NAME)



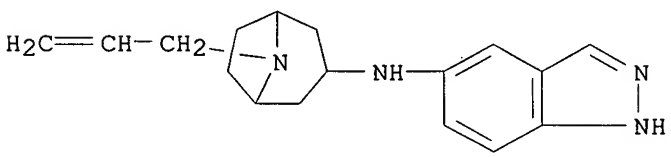
RN 478836-81-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-acetamide, 3-(1H-indazol-5-ylamino)- (9CI) (CA INDEX NAME)



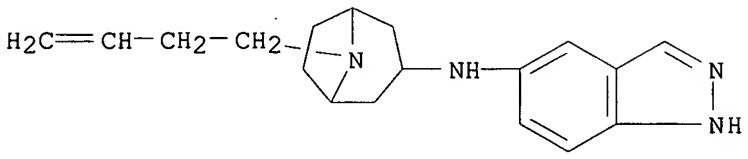
RN 478837-69-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-ethyl-N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



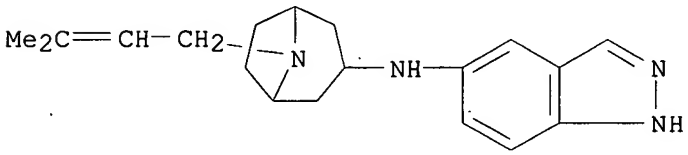
RN 478837-71-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(2-propenyl)- (9CI) (CA INDEX NAME)



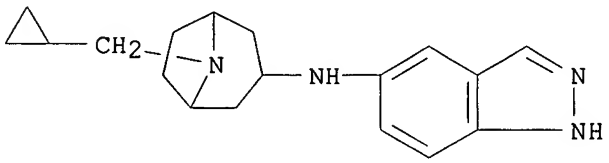
RN 478837-73-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-(3-butenyl)-N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



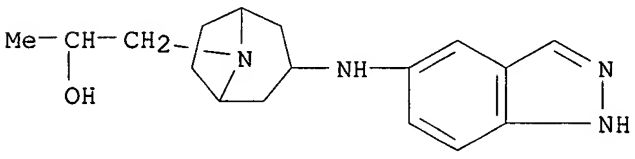
RN 478837-75-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)



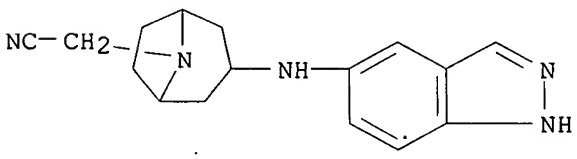
RN 478837-77-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-(cyclopropylmethyl)-N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



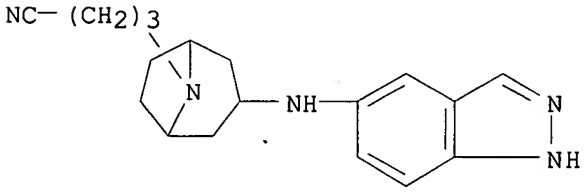
RN 478837-79-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-ethanol, 3-(1H-indazol-5-ylamino)-α-methyl- (9CI) (CA INDEX NAME)



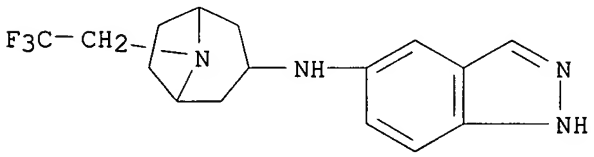
RN 478837-82-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-acetonitrile, 3-(1H-indazol-5-ylamino)- (9CI) (CA INDEX NAME)



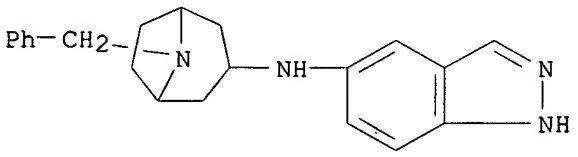
RN 478837-84-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-butanenitrile, 3-(1H-indazol-5-ylamino)- (9CI) (CA INDEX NAME)



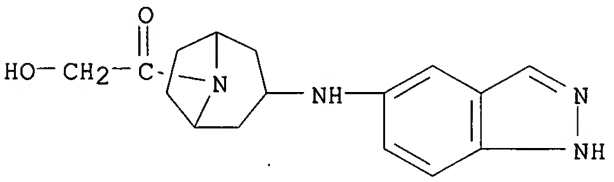
RN 478837-86-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)



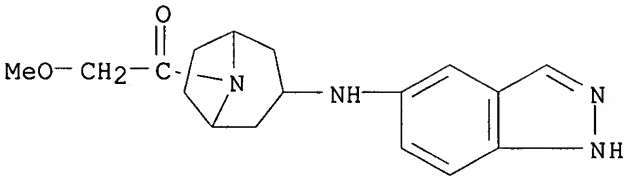
RN 478837-90-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(phenylmethyl)- (9CI) (CA INDEX NAME)



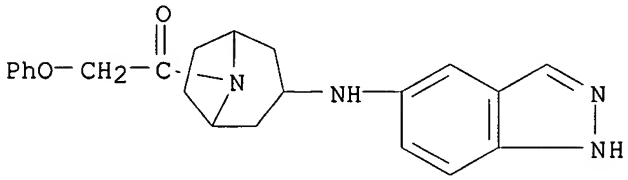
RN 478838-01-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-(hydroxyacetyl)-N-1H-indazol-5-yl- (9CI) (CA INDEX NAME)



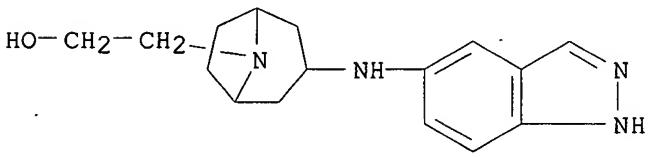
RN 478838-04-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(methoxyacetyl)- (9CI) (CA INDEX NAME)



RN 478838-06-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-(phenoxyacetyl)-(9CI) (CA INDEX NAME)

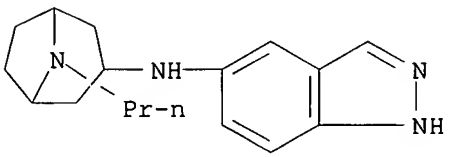


RN 478838-10-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-ethanol, 3-(1H-indazol-5-ylamino)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

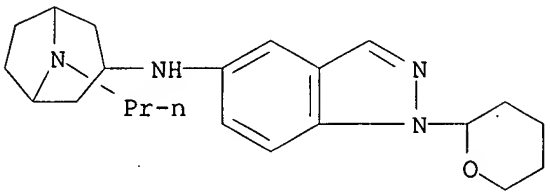
RN 478838-12-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-1H-indazol-5-yl-8-propyl-, dihydrochloride (9CI) (CA INDEX NAME)



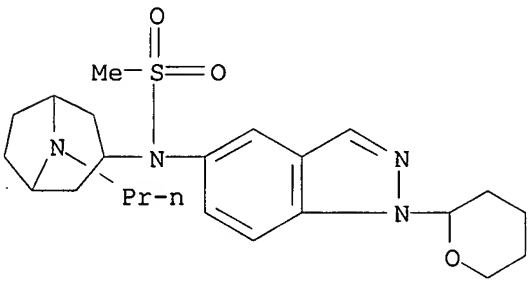
●2 HCl

IT 478837-61-5P, N-(8-Propyl-8-azabicyclo[3.2.1]oct-3-yl)-1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-amine 478837-62-6P, N-(8-Propyl-8-azabicyclo[3.2.1]oct-3-yl)-N-(1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-yl)-methanesulfonamide 478837-64-8P, N-(8-Propyl-8-azabicyclo[3.2.1]oct-3-yl)-N-(1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-yl)-acetamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic compds. as Rho-kinase inhibitors)

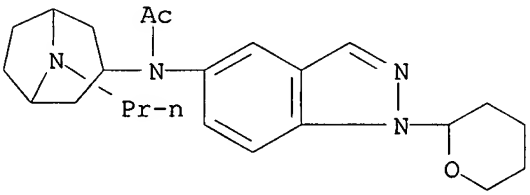
RN 478837-61-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-propyl-N-[1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-yl]- (9CI) (CA INDEX NAME)



RN 478837-62-6 CAPLUS
CN Methanesulfonamide, N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)-N-[1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-yl]- (9CI) (CA INDEX NAME)



RN 478837-64-8 CAPLUS
CN Acetamide, N-(8-propyl-8-azabicyclo[3.2.1]oct-3-yl)-N-[1-(tetrahydro-2H-pyran-2-yl)-1H-indazol-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

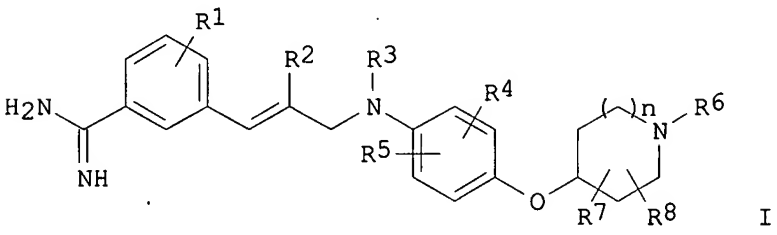
L5 ANSWER 3 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:868737 CAPLUS
DOCUMENT NUMBER: 137:369982
TITLE: Preparation of 2-[3-[4-(4-piperidinyloxy)anilino]-1-propenyl]benzamidine derivatives and composition containing them for iontophoresis
INVENTOR(S): Fujimoto, Koichi; Tanaka, Naoki; Shimada, Ikuko; Asai, Fumitoshi; Inoue, Kazuhiro; Okada, Junichi
PATENT ASSIGNEE(S): Sankyo Company, Limited, Japan
SOURCE: PCT Int. Appl., 400 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2002089803	A1	20021114	WO 2002-JP4422	20020507 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002253683	A1	20021118	AU 2002-253683	20020507 <--
JP 2003040773	A	20030213	JP 2002-131052	20020507
PRIORITY APPLN. INFO.:			JP 2001-136159	A 20010507
			WO 2002-JP4422	W 20020507

OTHER SOURCE(S): MARPAT 137:369982

GI



I

AB An iontophoresis composition for blood clotting factor X inhibitors which contains either a benzamidine derivative having the general formula (I) [wherein R1 = H, halo, alkyl, HO; R2 = H, halo, C1-6 alkyl; R3 = H, C1-6 alkyl, C1-6 hydroxyalkyl, C2-7 carboxyalkyl, C3-13 alkoxycarbonylalkyl, C7-16 aralkyl, C2-7 aliphatic acyl, C2-7 hydroxy-aliphatic acyl, C1-6 alkylsulfonyl, C3-13 alkoxycarbonylalkylsulfonyl, C2-7 carboxyalkylsulfonyl, C3-8 carboxyalkylcarbonyl; R4, R5 = H, halo, C1-6 alkyl, C1-6 haloalkyl, C1-6 alkoxy, CO2H, C2-7 alkoxycarbonyl, CONH2, C2-7 monoalkyl or C3-13 dialkylcarbamoyl; R6 = H, C1-6 alkyl, C3-8 cycloalkyl, C7-16 aralkyl, heterocyclyl-C1-6 alkyl, C2-7 carboxyalkyl, C3-13 alkoxycarbonylalkyl, C2-7 aliphatic acyl, C7-11 aromatic acyl, CONH2, C1-6 alkylsulfonyl, C6-10 aryl, heterocyclyl, formimidoyl, C2-7 1-iminoalkyl, C2-7 N-alkylformimidoyl, C7-11 iminoarylmethyl; R7, R8 = H, C1-6 alkyl; or R6 and R7 or R7 and R8 together represent C2-5 alkylene; n = 0, 1,2] or a pharmacol. acceptable salt of the derivative is disclosed. The compds. I are readily absorbed through skin and useful as remedies or preventives for thrombus or embolus by iontophoresis. Thus, 0.39 g Et acetimidate hydrochloride and 0.87 mL Et3N were added to a solution of [N-[(E)-3-(3-amidinophenyl)-2-methyl-2-propenyl]-N-[3-carbamoyl-4-(piperidin-4-yloxy)phenyl]sulfamoyl]acetic acid Et ester in 20 mL ethanol and stirred at room temperature for 6 h to give 75% [N-[4-((1-acetimidoylpiperidin-4-yl)oxy)-3-carbamoyl-N-[(E)-3-(3-amidinophenyl)-2-methyl-2-propenyl]phenyl]sulfamoyl]acetic acid Et ester dihydrochloride which (0.64 g) was dissolved in 20 mL 3 N aqueous HCl and heated at 80° for 2 h to give [N-[4-((1-acetimidoylpiperidin-4-yl)oxy)-3-carbamoylphenyl]-N-[(E)-3-(3-amidinophenyl)-2-methyl-2-propenyl]sulfamoyl]acetic acid dihydrochloride (II). II in vitro exhibited an iontophoresis skin permeability (flux) of 90±7 μg/h/cm2 using a hairless mice skin at skin current of 100 μA/cm2. The 15 compds. I exhibited higher skin permeability compared to two reference compds.

IT 470690-52-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

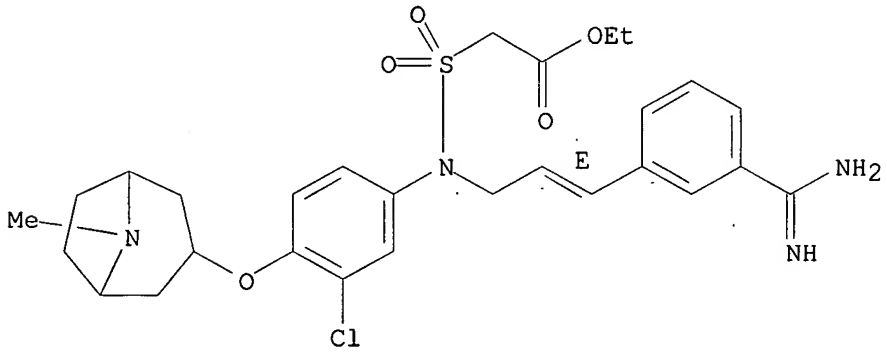
(preparation of [[(piperidinyloxy)anilino]propenyl]benzamidine derivs. as

blood clotting factor X inhibitors for treatment of thrombus and embolus by iontophoresis)

RN 470690-52-9 CAPLUS

CN Acetic acid, [[[(2E)-3-[3-(aminoiminomethyl)phenyl]-2-propenyl][3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl]amino]sulfonyl]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.



●2 HCl

IT 470690-53-0P

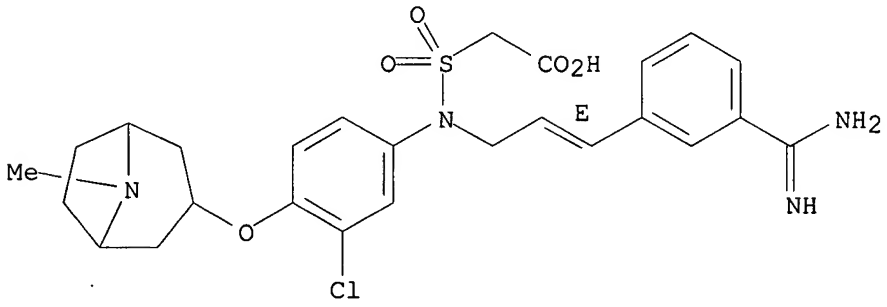
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of [[(piperidinyloxy)anilino]propenyl]benzamidine derivs. as blood clotting factor X inhibitors for treatment of thrombus and embolus by iontophoresis)

RN 470690-53-0 CAPLUS

CN Acetic acid, [[[(2E)-3-[3-(aminoiminomethyl)phenyl]-2-propenyl][3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl]amino]sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.



●2 HCl

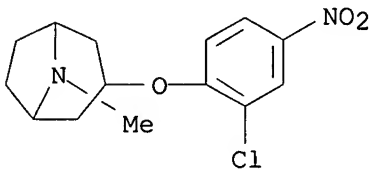
IT 470477-80-6P, 3-Chloro-4-[(tropan-3-yl)oxy]nitrobenzene
470477-81-7P, 3-Chloro-4-[(tropan-3-yl)oxy]aniline
470477-82-8P, [N-[3-Chloro-4-[(tropan-3-yl)oxy]phenyl]sulfamoyl]acetic acid ethyl ester 470690-54-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [[(piperidinyloxy)anilino]propenyl]benzamidine derivs. as blood clotting factor X inhibitors for treatment of thrombus and embolus by iontophoresis)

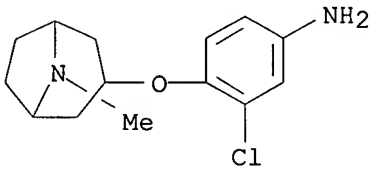
RN 470477-80-6 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-(2-chloro-4-nitrophenoxy)-8-methyl- (9CI) (CA INDEX NAME)



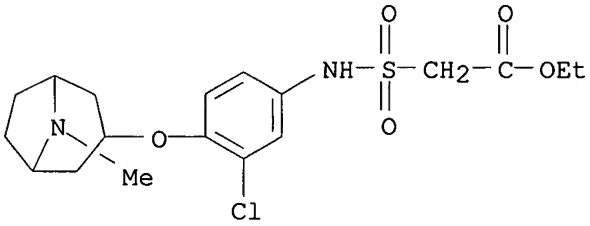
RN 470477-81-7 CAPLUS

CN Benzenamine, 3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]- (9CI) (CA INDEX NAME)



RN 470477-82-8 CAPLUS

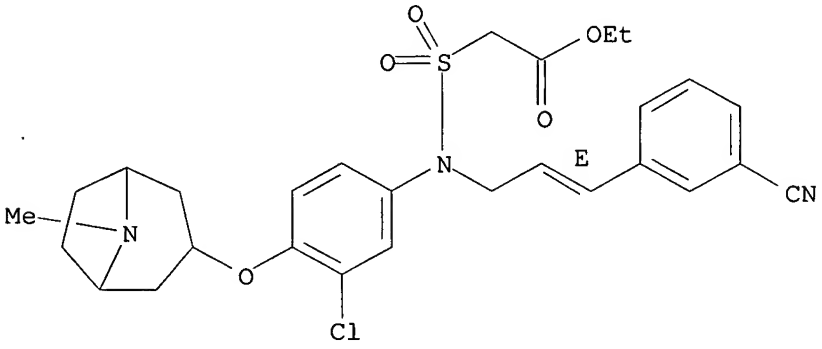
CN Acetic acid, [[[3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl]amino]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 470690-54-1 CAPLUS

CN Acetic acid, [[[(2E)-3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl][3-(3-cyanophenyl)-2-propenyl]amino]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



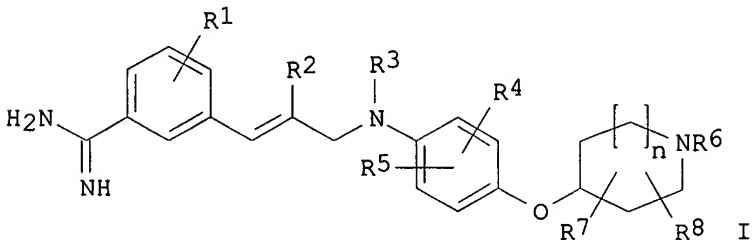
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:793603 CAPLUS
DOCUMENT NUMBER: 137:310926
TITLE: Preparation of benzamidine derivatives as inhibitors of activated blood coagulation factor X
INVENTOR(S): Fujimoto, Koichi; Tanaka, Naoki; Shimada, Ikuko; Asai, Fumitoshi
PATENT ASSIGNEE(S): Sankyo Company, Limited, Japan
SOURCE: PCT Int. Appl., 314 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002081448	A1	20021017	WO 2002-JP3355	20020403 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2442904	A1	20021017	CA 2002-2442904	20020403 <--
AU 2002246336	A1	20021021	AU 2002-246336	20020403 <--
EP 1375482	A1	20040102	EP 2002-714444	20020403
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002008678	A	20040330	BR 2002-8678	20020403
NZ 528517	A	20040827	NZ 2002-528517	20020403
HU 200400384	A2	20040928	HU 2004-384	20020403
CN 1610666	A	20050427	CN 2002-811105	20020403
RU 2256652	C1	20050720	RU 2003-129502	20020403
JP 2002363159	A	20021218	JP 2002-102486	20020404 <--
IN 2003KN01213	A	20050930	IN 2003-KN1213	20030922
ZA 2003007646	A	20040713	ZA 2003-7646	20030930
NO 2003004439	A	20031202	NO 2003-4439	20031003
US 2004147555	A1	20040729	US 2003-679215	20031003
US 7030138	B2	20060418		

PRIORITY APPLN. INFO.: JP 2001-107615 A 20010405
WO 2002-JP3355 W 20020403

OTHER SOURCE(S): MARPAT 137:310926
GI



I

AB The title compds. I [R1 represents a hydrogen atom, a halogen atom, an

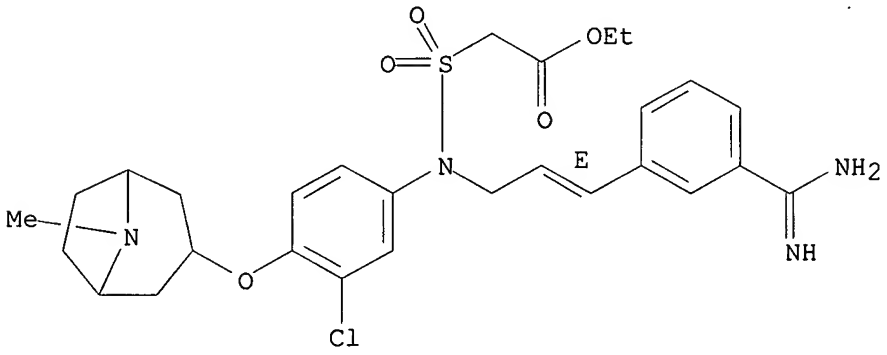
alkyl group or a hydroxyl group, R2 represents a hydrogen atom or a halogen atom, R3 represents a hydrogen atom, an alkyl group optionally substituted, an aralkyl group, an alkylcarbonyl group optionally substituted, an alkylsulfonyl group optionally substituted, or the like, R4 and R5 each represent a hydrogen atom, a halogen atom, an alkyl or carbamoyl group optionally substituted, or the like, R6 represents a hetero-ring or the like, R7 and R8 each represent a hydrogen atom, an alkyl group, or the like, and n represents 0,1 or 2] are prepared I are useful in the therapy or prevention of blood coagulation diseases. Compds. of this invention in vitro showed IC50 values of 5.8 nM to 15 nM against factor Xa. Formulations are given.

IT 470690-52-9P, N-[3-(3-Amidinophenyl)-2-(E)-propenyl]-N-[3-chloro-4-(tropan-3-yloxy)phenyl]sulfamoylacetic acid ethyl ester dihydrochloride
470690-53-0P, N-[3-(3-Amidinophenyl)-2-(E)-propenyl]-N-[3-chloro-4-(tropan-3-yloxy)phenyl]sulfamoylacetic acid dihydrochloride
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzamidine derivs. as inhibitors of activated blood coagulation factor X)

RN 470690-52-9 CAPLUS

CN Acetic acid, [[[(2E)-3-[3-(aminoiminomethyl)phenyl]-2-propenyl][3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl]amino]sulfonyl]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

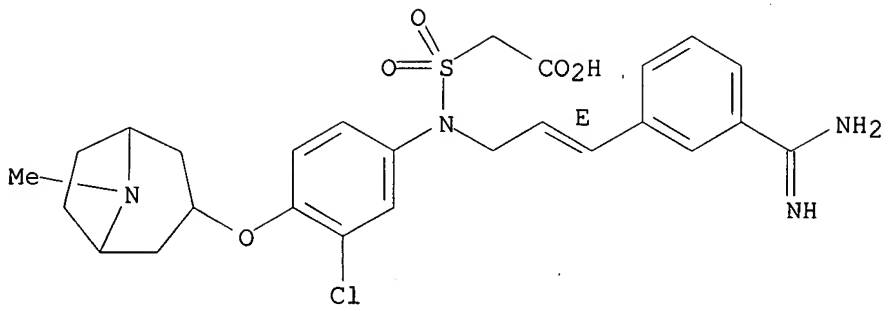


●2 HCl

RN 470690-53-0 CAPLUS

CN Acetic acid, [[[(2E)-3-[3-(aminoiminomethyl)phenyl]-2-propenyl][3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl]amino]sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

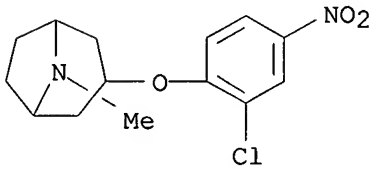
Double bond geometry as shown.



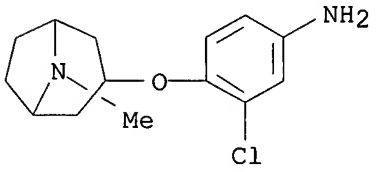
● 2 HCl

IT 470477-80-6P, 3-Chloro-4-(tropan-3-yloxy)nitrobenzene
470477-81-7P, 3-Chloro-4-(tropan-3-yloxy)aniline
470477-82-8P, N-[3-Chloro-4-(tropan-3-yloxy)phenyl]sulfamoylacetic acid ethyl ester 470690-54-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzamidine derivs. as inhibitors of activated blood coagulation factor X)

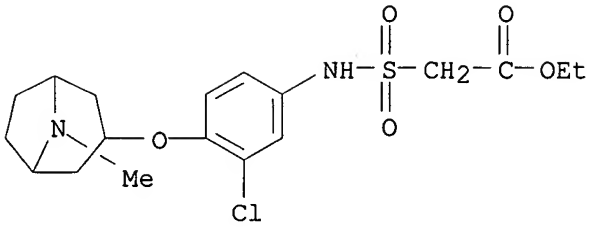
RN 470477-80-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane, 3-(2-chloro-4-nitrophenoxy)-8-methyl- (9CI) (CA INDEX NAME)



RN 470477-81-7 CAPLUS
CN Benzenamine, 3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]- (9CI) (CA INDEX NAME)

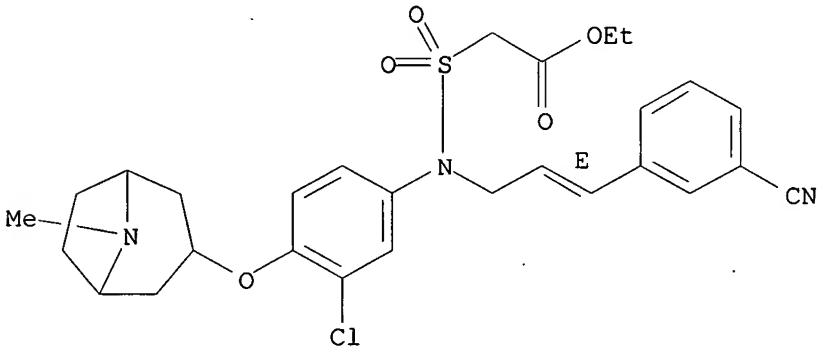


RN 470477-82-8 CAPLUS
CN Acetic acid, [[[3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl]amino]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



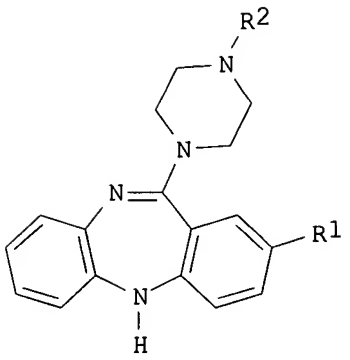
RN 470690-54-1 CAPLUS
CN Acetic acid, [[[(2E)-3-chloro-4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]phenyl][3-(3-cyanophenyl)-2-propenyl]amino]sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

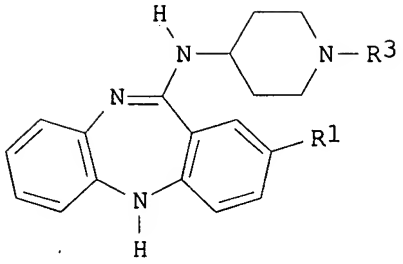


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:760723 CAPLUS
DOCUMENT NUMBER: 138:24701
TITLE: New Pyridobenzodiazepine Derivatives: Modifications of the Basic Side Chain Differentially Modulate Binding to Dopamine (D4.2, D2L) and Serotonin (5-HT2A) Receptors
AUTHOR(S): Liegeois, Jean-Francois; Eyrolles, Laurence; Ellenbroek, Bart A.; Lejeune, Christel; Carato, Pascal; Bruhwyler, Jacques; Geczy, Joseph; Damas, Jacques; Delarge, Jacques
CORPORATE SOURCE: Natural and Synthetic Drugs Research Center, Laboratory of Medicinal Chemistry, University of Liege, Liege, B-4000, Belg.
SOURCE: Journal of Medicinal Chemistry (2002), 45(23), 5136-5149
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:24701
GI



I



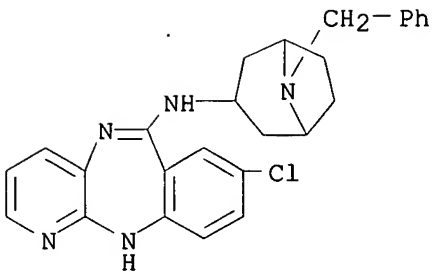
II

AB A series of new pyridobenzodiazepines with variation of the basic side chain were synthesized and evaluated for their binding to D4.2, D2L, and 5-HT2A receptors in comparison with clozapine, haloperidol, and two parent compds. previously described, 8-chloro-6-(4-methyl-1-piperazinyl)-11H-pyrido[2,3-b][1,4]benzodiazepine and 8-methyl-6-(4-methyl-1-piperazinyl)-11H-pyrido[2,3-b][1,4]benzodiazepine. In the piperazine series, replacing the N-Me group by a N-Ph moiety, as in I [R1 = Cl, Me; R2 = Ph, 3-ClC6H4, 3-CF3C6H4, PhCH2, Ph(CH2)2], provided a dramatic decrease of affinity for all receptors (Ki > 1000 nM). A N-cyclohexyl group restored some affinity. Compds. with a N-benzyl or N-phenethyl side chain had significant affinities at D4.2 and 5-HT2A receptors. Homologation of the piperazine nucleus led to a significant decrease of the affinity at all receptors investigated. In the 4-aminopiperidine series, N-Me derivs. II [R1 = Cl, Me; R3 = Me] possessed less affinity in comparison with the N-methylpiperazine analogs while the N-benzyl congeners showed similar affinities. The rigidification of piperidine nucleus as obtained in azabicyclo[3.2.1]octane derivs. involved a slight reduction of the affinity at D4.2 and 5-HT2A receptors while the affinity at D2L receptors was dramatically increased. The introduction of N-substituted aminoalkylamines to replace N-methylpiperazine generally led to a significant decrease in the affinity for D4.2 receptors but some of these mols. (24, 25, 41) presented a significant 5-HT2A binding affinity. The presence of a more flexible side chain induced an increased conformational freedom. Consequently, the preferential position of the distal nitrogen or its basicity in piperazine derivs. was greatly modified. I [R1 = Cl, R2 = Ph(CH2)2] with a high D4.2 and 5-HT2A affinity (Ki = 40 and 103 nM, resp.) did not induce cataleptic phenomenon in the paw test in rats but significantly reduced the immobility time in Porsolt's test in mice suggesting antidepressant properties.

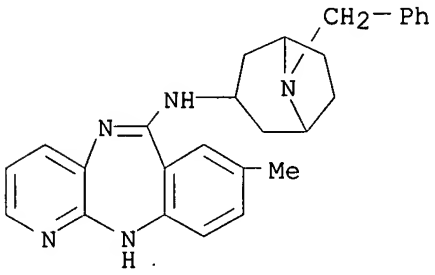
IT 478166-83-5P 478166-99-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, structure-activity relationship, and in vitro affinities and binding ratio to α-adrenoreceptors, dopamine and serotonin receptors of pyridobenzodiazepines)

RN 478166-83-5 CAPLUS

CN 1H-Pyrido[2,3-b][1,4]benzodiazepin-6-amine, 8-chloro-N-[8-(phenylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]- (9CI) (CA INDEX NAME)



RN 478166-99-3 CAPLUS
CN 1H-Pyrido[2,3-b][1,4]benzodiazepin-6-amine, 8-methyl-N-[8-(phenylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:574925 CAPLUS
DOCUMENT NUMBER: 137:140442
TITLE: Preparation of 1,5-diaryl-7-heterocyclyl(alkyl)-2-quinolinones as p38 protein kinase inhibitors
INVENTOR(S): Doherty, James B.; Stelmach, John E.; Chen, Meng-Hsin; Liu, Luping; Hunt, Julianne A.; Ruzek, Rowena D.; Goulet, Joung L.; Wisnoski, David D.; Natarajan, Swaminathan Ravi; Rupprecht, Kathleen M.; Bao, Jianming; Miao, Shouwu; Hong, Xingfang
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 440 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

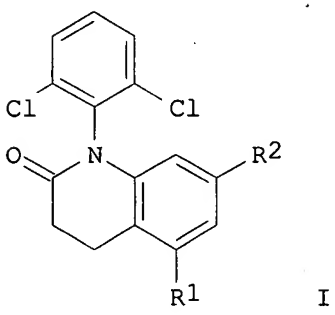
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058695	A1	20020801	WO 2001-US48676	20011214 <--
WO 2002058695	A9	20030912		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2431904	A1	20020801	CA 2001-2431904		20011214 <--
AU 2002246677	A1	20020806	AU 2002-246677		20011214 <--
EP 1345603	A1	20030924	EP 2001-994260		20011214
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004521892	T	20040722	JP 2002-559029		20011214
US 2003092712	A1	20030515	US 2001-23231		20011217
US 6809199	B2	20041026			
PRIORITY APPLN. INFO.:			US 2000-256822P	P	20001220
			WO 2001-US48676	W	20011214

OTHER SOURCE(S): MARPAT 137:140442

GI



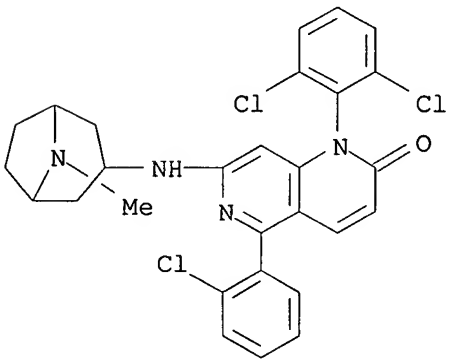
I

AB Title compds. were prepared Thus, 2,6-dibromo-4-methoxytoluene was converted in 5 steps to arylquinolinone I (R1 = Br, R2 = OMe) which was condensed with 2,4-F2C6H3B(OH)2 and the O-demethylated product converted in 4 steps to I (R1 = C6H3F2-2,4, R2 = 4-piperidinyl). Data for biol. activity of title compds. were given.

IT 444661-83-0P 444661-94-3P 444766-00-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,5-diaryl-7-heterocyclyl(alkyl)-2-quinolinones as p38 protein kinase inhibitors)

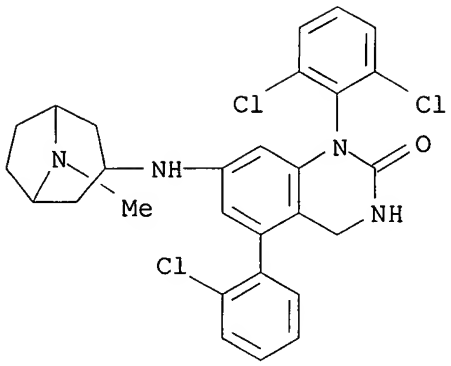
RN 444661-83-0 CAPLUS

CN 1,6-Naphthyridin-2(1H)-one, 5-(2-chlorophenyl)-1-(2,6-dichlorophenyl)-7-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)amino]- (9CI) (CA INDEX NAME)

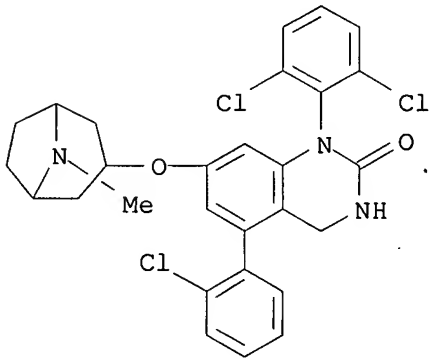


RN 444661-94-3 CAPLUS

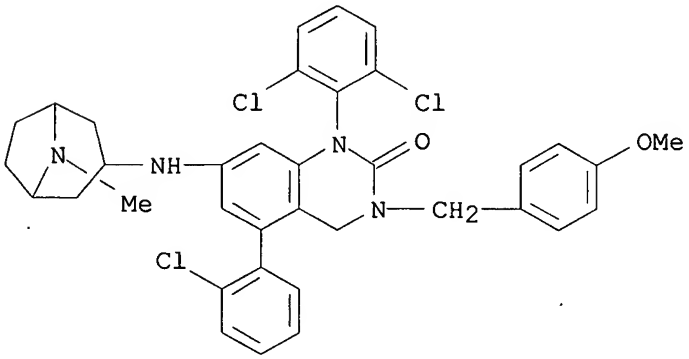
CN 2(1H)-Quinazolinone, 5-(2-chlorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)amino]- (9CI) (CA INDEX NAME)



RN 444766-00-1 CAPLUS
CN 2(1H)-Quinazolinone, 5-(2-chlorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-7-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]- (9CI) (CA INDEX NAME)



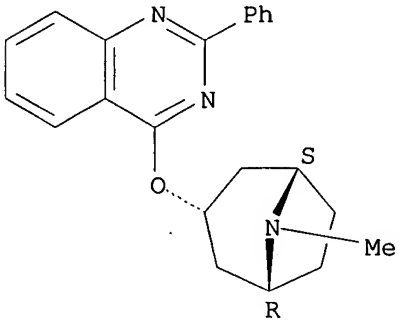
IT 444665-73-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,5-diaryl-7-heterocyclyl(alkyl)-2-quinolinones as p38 protein kinase inhibitors)
RN 444665-73-0 CAPLUS
CN 2(1H)-Quinazolinone, 5-(2-chlorophenyl)-1-(2,6-dichlorophenyl)-3,4-dihydro-3-[(4-methoxyphenyl)methyl]-7-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:543678 CAPLUS
DOCUMENT NUMBER: 138:106650
TITLE: Identification of a novel partial inhibitor of dopamine transporter among 4-substituted 2-phenylquinazolines
AUTHOR(S): Ananthan, Subramaniam; Saini, Surendra K.; Khare, Rashmi; Clayton, Sarah D.; Dersch, Christina M.; Rothman, Richard B.
CORPORATE SOURCE: Organic Chemistry Department, Southern Research Institute, Birmingham, AL, 35255, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(16), 2225-2228
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:106650
AB In an attempt to identify novel ligands for the dopamine transporter, a series of 4-substituted-2-phenylquinazolines were synthesized and evaluated. Among the compds. studied, 4-[(diphenylmethyl)amino]-2-phenylquinazoline was identified as a novel partial inhibitor of [125I]RTI-55 binding to the dopamine transporter and a partial inhibitor of [3H]dopamine uptake.
IT 488081-99-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of 4-substituted 2-phenylquinazolines as partial inhibitors of dopamine transporter)
RN 488081-99-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane, 8-methyl-3-[(2-phenyl-4-quinazolinyl)oxy]-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:502824 CAPLUS
DOCUMENT NUMBER: 137:63122
TITLE: Preparation of purine derivatives or therapeutic use as phosphodiesterase IV inhibitors
INVENTOR(S): Chasin, Mark; Cavalla, David J.; Hofer, Peter; Gehrig, Andre; Wintergerst, Peter
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg
SOURCE: U.S., 34 pp., Cont.-in-part of U.S. Ser. No. 285,473.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

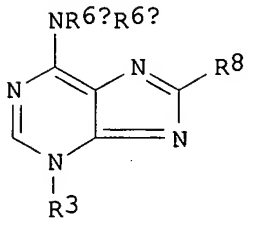
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6413975	B1	20020702	US 2000-539571	20000331 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
HU 200200938	A2	20021028	HU 2002-938	20000331 <--
JP 2001316314	A	20011113	JP 2000-136383	20000509 <--
US 2003073834	A1	20030417	US 2002-62280	20020201

PRIORITY APPLN. INFO.:

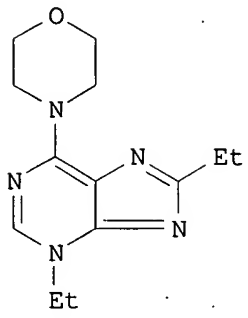
US 1999-285473 A2 19990402
IN 1994-CA514 A1 19940630
US 1997-963054 A2 19971103
US 1997-875487 A2 19971113
US 1998-151949 A2 19980911
US 1998-210556 A2 19981211
US 1998-210557 A2 19981211
US 1999-227057 A2 19990107
US 1999-237638 A2 19990126
US 1999-361196 A2 19990726
US 2000-506624 A2 20000218
US 2000-539571 A2 20000331
US 2000-547575 A2 20000412
US 2000-547898 A2 20000412
US 2000-636146 A2 20000810
US 2000-724321 B1 20001128

OTHER SOURCE(S): MARPAT 137:63122

GI



I



II

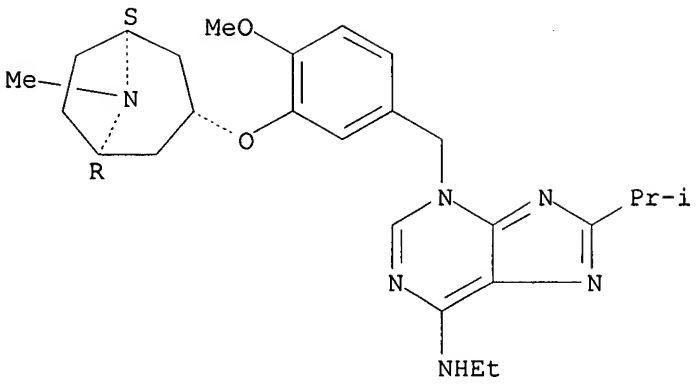
AB Purines, such as I [R3, R6a, R6b, R8 = H, alkyl, alkenyl, cycloalkyl, aryl, arylalkyl, etc.], were prepared for pharmaceutical use as phosphodiesterase IV (PDE IV) inhibitors. Thus, 3,8-diethyl-6-morpholino-3H-purine (II) was prepared by conversion of 3,8-diethyl-2-thioxanthine to 3,8-diethylhypoxanthine using 2N NaOH and nickel aluminum alloy, reaction of 3,8-diethylhypoxanthine to 3,8-diethyl-6-thiohypoxanthine using phosphorus pentasulfide in pyridine and, finally, reaction of 3,8-diethyl-6-thiohypoxanthine with morpholine. The prepared purine derivs. were assayed for PDE IV inhibition.

IT 300784-31-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)

RN 300784-31-0 CAPLUS

CN 3H-Purin-6-amine, N-ethyl-3-[[4-methoxy-3-[[(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]oxy]phenyl]methyl]-8-(1-methylethyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

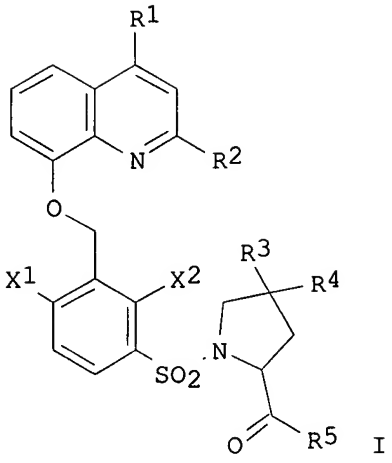


REFERENCE COUNT: 86 THERE ARE 86 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:446120 CAPLUS
DOCUMENT NUMBER: 137:33534
TITLE: Preparation of N-benzenesulfonyl-L-proline compounds as bradykinin antagonists
INVENTOR(S): Katsu, Yasuhiro; Kawai, Makoto; Koike, Hiroki; Nukui, Seiji
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 1213289	A1	20020612	EP 2001-310151	20011204	<--
EP 1213289	B1	20031105			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
CA 2364178	A1	20020605	CA 2001-2364178	20011203	<--
CA 2364178	C	20060110			
BR 2001005775	A	20020813	BR 2001-5775	20011204	<--
AT 253575	T	20031115	AT 2001-310151	20011204	
PT 1213289	T	20040130	PT 2001-310151	20011204	
ES 2208523	T3	20040616	ES 2001-1310151	20011204	
JP 2002220387	A	20020809	JP 2001-371430	20011205	<--
US 2002128271	A1	20020912	US 2001-10863	20011205	<--
US 6734306	B2	20040511			

PRIORITY APPLN. INFO.: US 2000-251225P P 20001205
OTHER SOURCE(S): MARPAT 137:33534
GI



I

AB Proline derivs. I [X1, X2 = halo or C1-4 alkyl; R1, R2 = H or C1-4 alkyl; R3, R4 = H or halo; R5 = C3-9 diazacycloalkyl optionally substituted with C5-11 azabicycloalkyl, C3-9 azacycloalkyl-NH-(C5-11 azabicycloalkyl optionally substituted with C1-4 alkyl), NH-C1-3 alkyl-C(O)-C5-11 diazabicycloalkyl, NH-C1-3 alkyl-C(O)-NH-C5-11 azabicycloalkyl, the C5-11 azabicycloalkyl being optionally substituted with C1-4 alkyl, C3-9 azacycloalkyl optionally substituted with C3-9 azacycloalkyl, or NH-C1-5 alkyl-NHC(O)-C4-9 cycloalkyl-NH] or their pharmaceutically-acceptable salts were prepared for the treatment of medical conditions mediated by bradykinin, e.g., inflammation, allergic rhinitis, and pain. Thus, 8-[[3-[[(2S)-2-[[4-[(3S)-1-azabicyclo[2.2.2]oct-3-yl]-1-piperazinyl]carbonyl]pyrrolidinyl]sulfonyl]-2,6-dichlorobenzyl]oxy]-2,4-dimethylquinoline hydrochloride was prepared via acylation of 3(S)-(1-piperazinyl)-1-azabicyclo[2.2.2]octane (preparation given). The biol. activity of compds. of the invention was determined by their ability to inhibit the binding of bradykinin at its receptor sites in recombinant human bradykinin B2 receptor expressing CHO-K1 cells (IC50 values for the synthesized compds. were 0.1-4 nM).

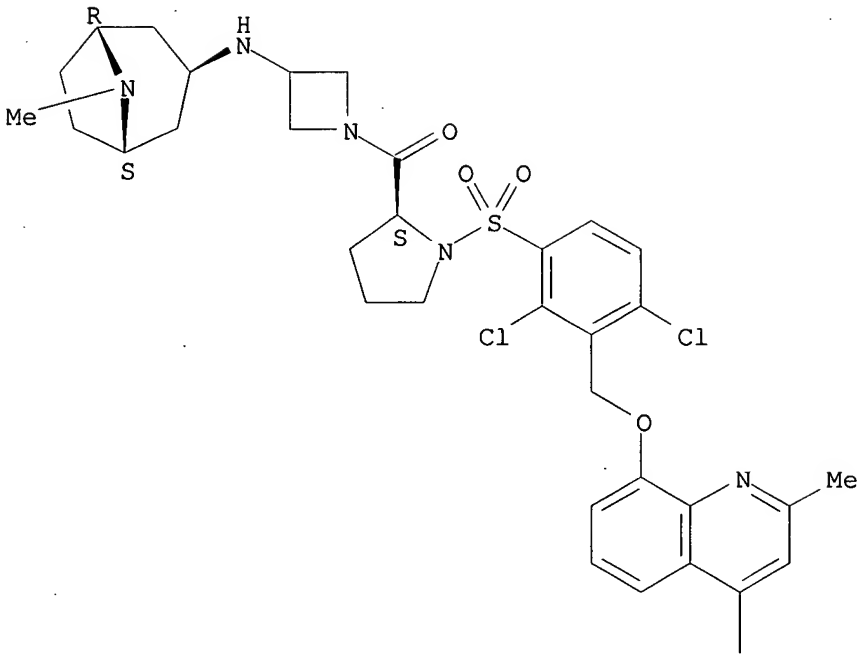
IT 436099-26-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-benzenesulfonyl-L-proline compds. as bradykinin antagonists)

RN 436099-26-2 CAPLUS

CN 3-Azetidinamine, 1-[[(2S)-1-[[2,4-dichloro-3-[[(2,4-dimethyl-8-quinolinyl)oxy]methyl]phenyl]sulfonyl]-2-pyrrolidinyl]carbonyl]-N-[(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

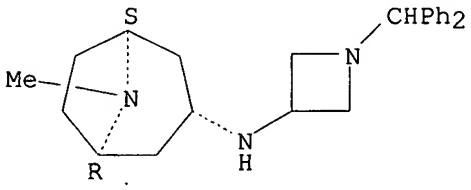


PAGE 2-A

IT 436099-35-3P 436099-36-4P 436099-37-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-benzenesulfonyl-L-proline compds. as bradykinin antagonists)

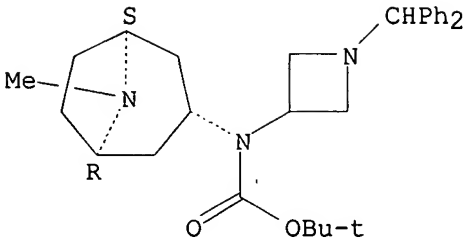
RN 436099-35-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-[1-(diphenylmethyl)-3-azetidinyl]-8-methyl-, (3-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



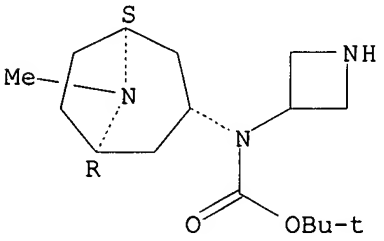
RN 436099-36-4 CAPLUS
CN Carbamic acid, [1-(diphenylmethyl)-3-azetidinyl][(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 436099-37-5 CAPLUS
CN Carbamic acid, 3-azetidinyl[(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

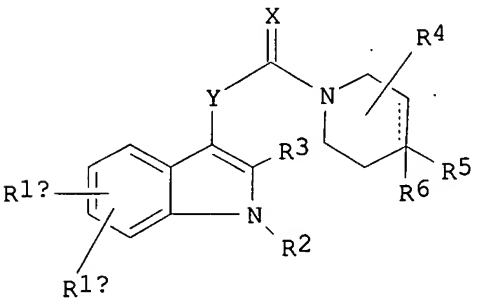


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:817246 CAPLUS
DOCUMENT NUMBER: 135:357843
TITLE: Preparation of 2-Aryl indole derivatives for use as tachykinin receptor antagonists
INVENTOR(S): Dinnell, Kevin; Elliott, Jason Matthew; Hollingworth, Gregory John; Ridgill, Mark Peter; Shaw, Duncan Edward
PATENT ASSIGNEE(S): UK
SOURCE: U.S. Pat. Appl. Publ., 37 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2001039286	A1	20011108	US 2001-782422		20010213 <--
PRIORITY APPLN. INFO.:			GB 2000-3397	A	20000214

OTHER SOURCE(S): MARPAT 135:357843
GI



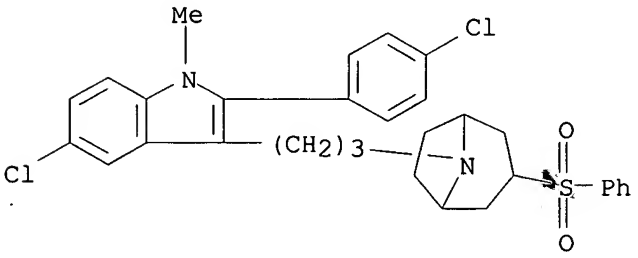
I

AB 2-Aryl indole derivs. I (wherein R1a, R1b, and R2 = a variety of substituents; R3 = optionally substituted Ph, biphenyl or naphthyl or heteroaryl group; R4 = H, (C1-6)alkyl, carbonyl (=O), (CH2)pphenyl or a (C1-2)alkylene bridge across the piperidine ring; R5 and R6 = variety of substituents; or R5 and R6 together are linked so as to form an optionally substituted 5-or 6-membered ring; X = O or S, two H atoms, boxHNH or boxHN(C1-6 alkyl); Y = straight or branched (C1-4)alkylene, (C2-4)alkenylene or (C2-4)alkynylene chain; the dotted line represents an optional double bond; m = 0,1,2,3,4; n = 1,2,3,4; and p = 1,2,3,4), or a pharmaceutically acceptable salt thereof, were prepared, and their use as tachykinin receptor antagonists evaluated. Thus, diisopropylethylamine and bromoacetonitrile were added to a loaded resin (synthetic preparation given) in N-methylpyrrolidinone, to which was added a solution of 6-(methylsulfonyl)spiro-[2H-1-benzopyran-2,4'-piperidin]-4(3H)-one in THF to give 1'-{3-[5-chloro-2-(4-chlorophenyl)-1H-indol-3-yl]-1-oxopropyl}-6-(methylsulfonyl)spiro(2H-1-benzopyran-2,4'-piperidin)-4(3H)-one. The compds. are of particular use in the treatment or prevention of depression, anxiety, pain, inflammation, migraine, emesis or postherpetic neuralgia. Biol. data are given.

IT 371970-31-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl indole derivs. as tachykinin receptor antagonists for treatment for)

RN 371970-31-9 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[3-[5-chloro-2-(4-chlorophenyl)-1-methyl-1H-indol-3-yl]propyl]-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)



=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	58.94	231.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.80	-7.80

FILE 'STNGUIDE' ENTERED AT 10:28:59 ON 15 MAY 2007

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 11, 2007 (20070511/UP).

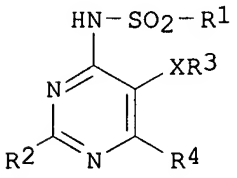
=> d ibib abs hitstr 11-20
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L5 ANSWER 11 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:798218 CAPLUS
DOCUMENT NUMBER: 135:331440
TITLE: Preparation of substituted sulfonylaminopyrimidines as endothelin receptor antagonists
INVENTOR(S): Boss, Christoph; Bolli, Martin; Clozel, Martine; Fischli, Walter; Weller, Thomas
PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd., Switz.
SOURCE: PCT Int. Appl., 124 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001081338	A1	20011101	WO 2001-EP4133	20010411 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: WO 2000-EP3692 W 20000425
OTHER SOURCE(S): MARPAT 135:331440
GI



I

AB The present invention relates to novel substituted pyrimidines I (e.g. rac-5-isopropyl-N-[5-(2-methoxyphenoxy)-2-(4-pyridyl)-6-(tetrahydrofuran-2-ylmethoxy)-4-pyrimidinyl]-2-pyridinesulfonamide) and pharmaceutically acceptable salts thereof and their use as active ingredients in the preparation of pharmaceutical compns. The invention also concerns related aspects including processes for the preparation of the compds., pharmaceutical compns. containing one or more I and especially their use as endothelin receptor antagonists. In I: R1 = aryl; aryl-lower alkyl; aryl-lower alkenyl; heteroaryl; heteroaryl-lower alkyl. R2 = H; halogen; trifluoromethyl; lower alkyl; lower alkylamino; lower alkyloxy; lower alkylsulfono; lower alkylsulfinyl; lower alkylthio; lower alkylthio-lower alkyl; hydroxy-lower alkyl; hydroxy-lower alkyloxy; lower alkyloxy-lower alkyl; lower alkyloxy-lower alkyloxy; hydroxy-lower alkyloxy-lower alkyl; hydroxy-lower alkyloxy-lower alkyloxy; lower alkyloxy-lower alkyloxy-lower alkyloxy; hydroxy-lower alkylamino; lower alkylamino-lower alkyl; amino; di-lower alkylamino; [N-(hydroxy-lower alkyl)-N-(lower alkyl)]amino; aryl; arylamino; aryl-lower alkylamino; arylthio; aryl-lower alkylthio; aryloxy. Also, R2 = aryl-lower alkyloxy; aryl-lower alkyl; arylsulfinyl; heteroaryl; heteroaryloxy; heteroaryl-lower alkyloxy; heteroarylamino; heteroaryl-lower alkylamino; heteroaryl-lower alkylthio; heteroaryl-lower alkyl; heteroarylsulfinyl; heterocyclyl; heterocyclyl-lower alkyloxy; heterocyclyloxy; heterocyclylamino; heterocyclyl-lower alkylamino;

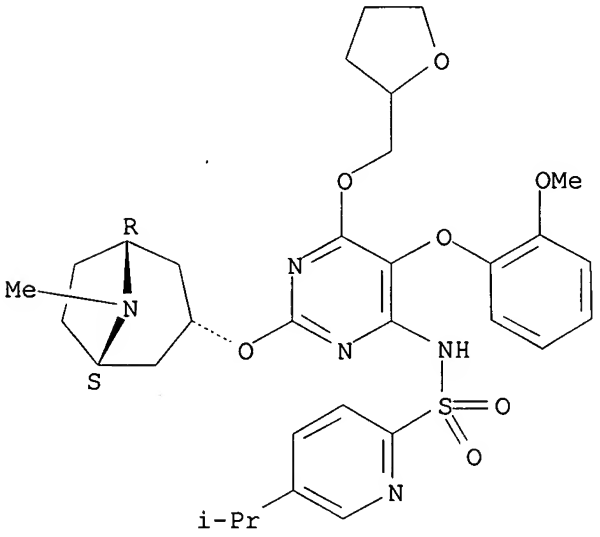
heterocyclylthio; heterocyclyl-lower alkylthio; heterocyclyl-lower alkyl; heterocyclylsulfinyl; cycloalkyl; cycloalkyloxy; cycloalkyl-lower alkyloxy; cycloalkylamino; cycloalkyl-lower alkylamino; cycloalkylthio; cycloalkyl-lower alkyl; cycloalkylsulfinyl; alkyloxycarbonyl; carboxy; cycloalkyl-lower alkylthio; cyano; aminocarbonyl. R3 = phenyl; mono, di- or trisubstituted Ph substituted with lower alkyl, lower alkenyl, lower alkyloxy, amino, lower alkylamino, amino-lower alkyl, trifluoromethyl, trifluoromethoxy, halogen, lower alkylthio, hydroxy, hydroxy-lower alkyl, cyano, carboxy, alkoxycarbonyl, lower alkanoyl, formyl; benzofuranyl; aryl; heteroaryl. X = O; S; NH; CH2 or a bond; R4 = N(CH2)2Z(CH2)2 (Z = = O, imino, S, SO, or SO2) and substituted alkoxy as specified in the claims. Ninety-two example prepns. are included, but the methods of preparation are not claimed. IC50 (concentration of antagonist inhibiting 50% of the specific binding of ET-1) values were determined for some of the claimed compds. and were as low as 6 nM (rac-5-methylpyridine-2-sulfonic acid [5-(2-methoxyphenoxy)-6-(tetrahydrofuran-2-ylmethoxy)-2-[2-(5-thioxo-4,5-dihydro-[1,2,4]oxadiazol-3-yl)pyridin-4-yl]pyrimidin-4-yl]amide). Also, pA2 (neg. value of logarithm of antagonist concentration that induces 2-fold shift in concentration of endothelin needed to get half-maximal contraction on isolated rat aortic rings or rat tracheal rings) are reported for 5 I.

IT 370105-58-1P, (1'R,3'S,5'S,2''R/S)-5-isopropylpyridine-2-sulfonic acid [5-(2-methoxyphenoxy)-2-(8'-methyl-8'-azabicyclo[3.2.1]oct-3'-yloxy)-6-(tetrahydrofuran-2''-ylmethoxy)pyrimidin-4-yl]amide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted sulfonylaminopyrimidines as endothelin receptor antagonists)

RN 370105-58-1 CAPLUS

CN 2-Pyridinesulfonamide, N-[5-(2-methoxyphenoxy)-2-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]oxy]-6-[(tetrahydro-2-furanyl)methoxy]-4-pyrimidinyl]-5-(1-methylethyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

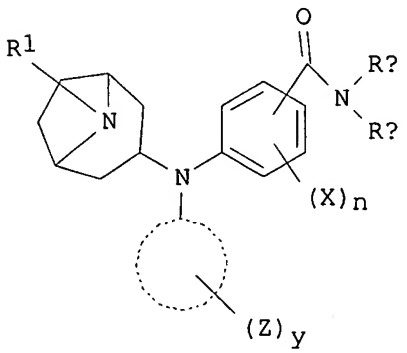
L5 ANSWER 12 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:730549 CAPLUS
DOCUMENT NUMBER: 135:283207
TITLE: Selective tropane ligands for the delta opioid receptor, their preparation and their therapeutic use

INVENTOR(S): Carroll, F. Ivy; Thomas, James B.; Mascarella, S. Wayne
PATENT ASSIGNEE(S): Research Triangle Institute, USA
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001072303	A1	20011004	WO 2001-US8629	20010329 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-537668 A 20000329
OTHER SOURCE(S): MARPAT 135:283207
GI

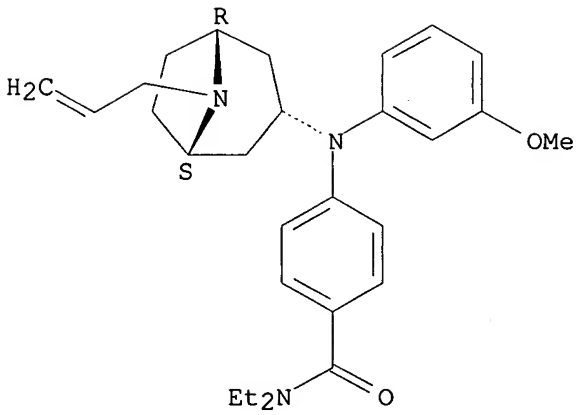


I

AB The invention discloses substituted tropane derivs. I [Ra, Rb = H, alkyl, alkenyl, or Ra and Rb bonded; X = alkyl; Z = alkyl, OH, OR, CF3, CN etc. ; R = alkyl, alkenyl, aryl, alkaryl; R1 = alkyl, alkenyl, alkaryl; n = 0-4; yr = 0-5; Z-substituted ring = 5 or 6 membered (hetero)aryl] which are selective for the delta opioid receptor. The invention also outlines the preparation of these derivs. e.g II (R1 = allyl) and their opioid receptor binding affinities. The inventive compds. may be used to treat disease states which are ameliorated by binding opioid receptors which include heroin addiction and pain (as analgesics).

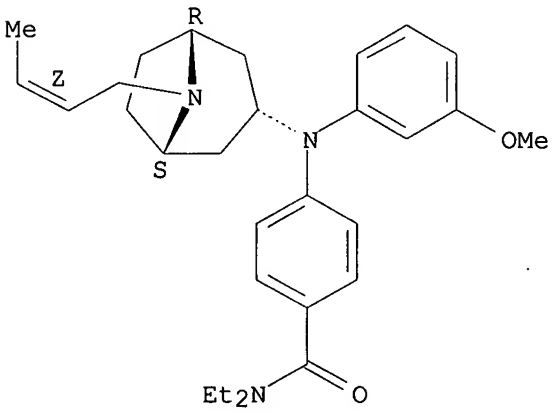
IT 289468-26-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(delta opioid receptor ligands, preparation and therapeutic use)
RN 289468-26-4 CAPLUS
CN Benzamide, N,N-diethyl-4-[(3-methoxyphenyl)[(3-endo)-8-(2-propenyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



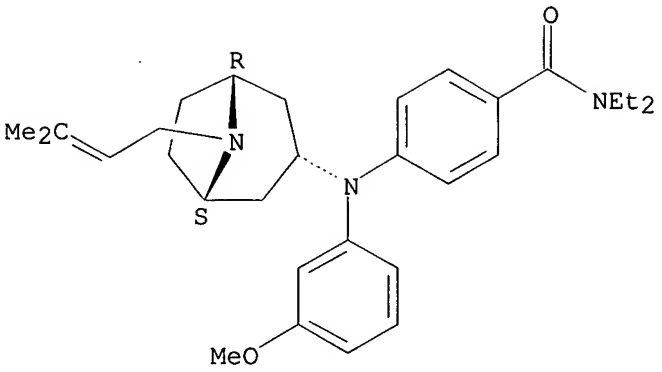
IT 289468-27-5P 289468-28-6P 289468-29-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(delta opioid receptor ligands, preparation and therapeutic use)
RN 289468-27-5 CAPLUS
CN Benzamide, 4-[[(3-endo)-8-(2Z)-2-butenyl-8-azabicyclo[3.2.1]oct-3-yl](3-methoxyphenyl)amino]-N,N-diethyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



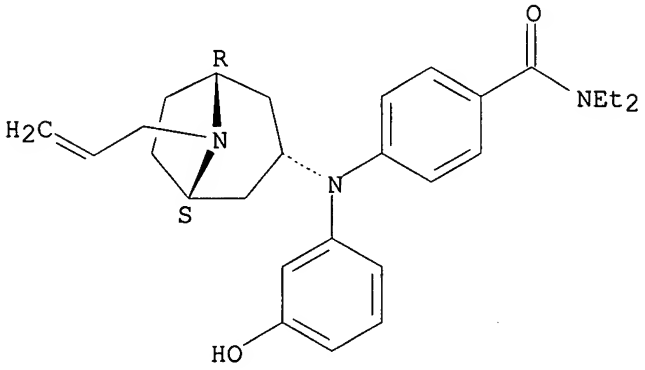
RN 289468-28-6 CAPLUS
CN Benzamide, N,N-diethyl-4-[(3-methoxyphenyl)[(3-endo)-8-(3-methyl-2-butenyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



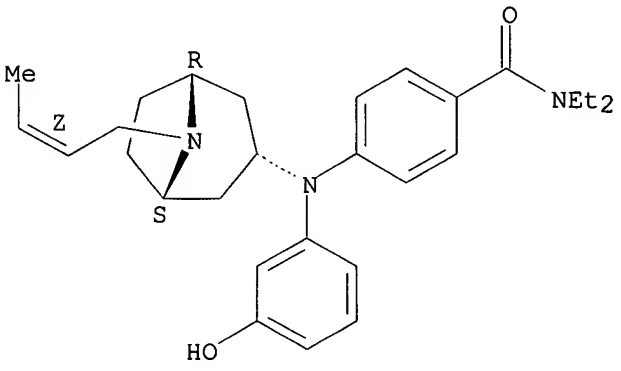
RN 289468-29-7 CAPLUS
CN Benzamide, N,N-diethyl-4-[(3-hydroxyphenyl)[(3-endo)-8-(2-propenyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 364039-21-4 364039-22-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(delta opioid receptor ligands, preparation and therapeutic use)
RN 364039-21-4 CAPLUS
CN Benzamide, 4-[[(3-endo)-8-(2Z)-2-butenyl-8-azabicyclo[3.2.1]oct-3-yl](3-hydroxyphenyl)amino]-N,N-diethyl- (9CI) (CA INDEX NAME)

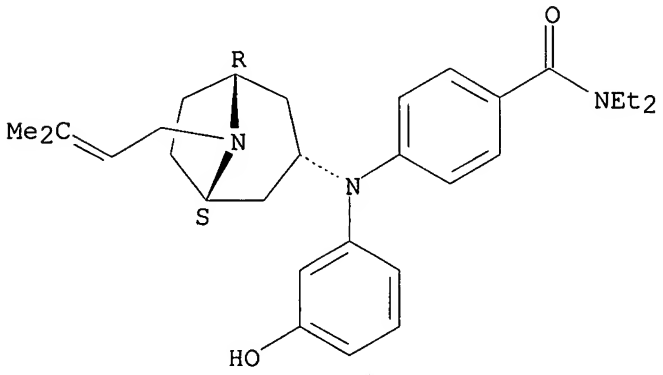
Relative stereochemistry.
Double bond geometry as shown.



RN 364039-22-5 CAPLUS

CN Benzamide, N,N-diethyl-4-[(3-hydroxyphenyl)[(3-endo)-8-(3-methyl-2-butenyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

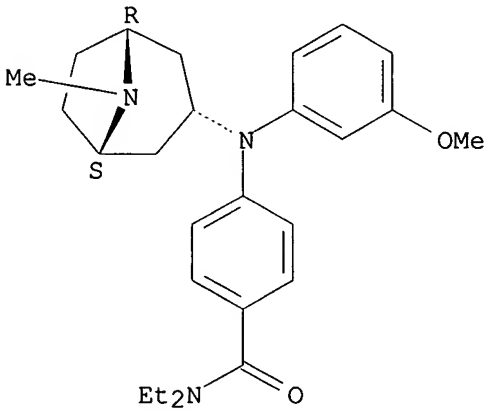
Relative stereochemistry.



IT 287720-99-4P 289468-30-0P 289468-31-1P
364039-20-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(delta opioid receptor ligands, preparation and therapeutic use)

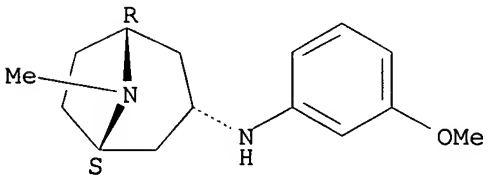
RN 287720-99-4 CAPLUS
CN Benzamide, N,N-diethyl-4-[(3-methoxyphenyl)[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 289468-30-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-(3-methoxyphenyl)-8-methyl-, (3-endo)- (9CI) (CA INDEX NAME)

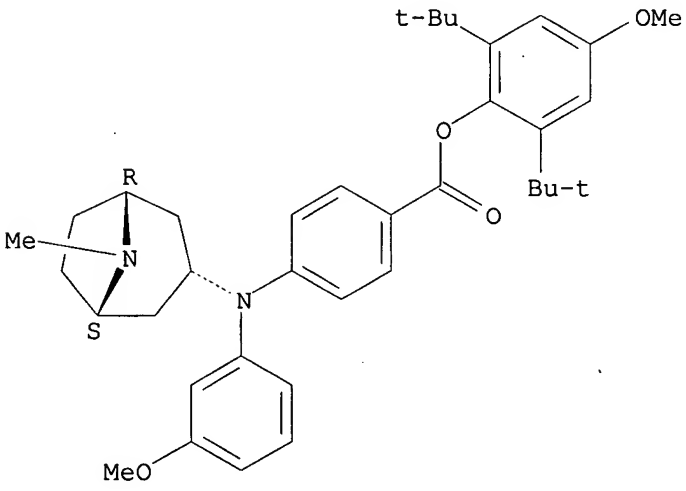
Relative stereochemistry.



RN 289468-31-1 CAPLUS
CN Benzoic acid, 4-[(3-methoxyphenyl)[(3-endo)-8-methyl-8-

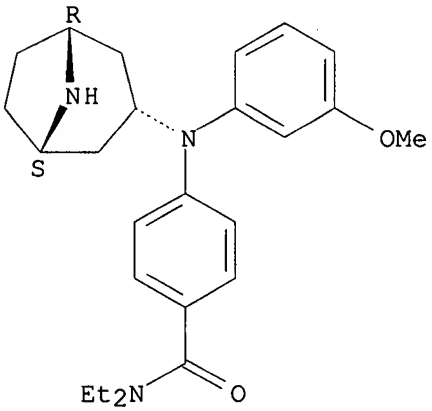
azabicyclo[3.2.1]oct-3-yl]amino]-, 2,6-bis(1,1-dimethylethyl)-4-methoxyphenyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 364039-20-3 CAPLUS
CN Benzamide, 4-[(3-endo)-8-azabicyclo[3.2.1]oct-3-yl(3-methoxyphenyl)amino]-N,N-diethyl- (9CI) (CA INDEX NAME)

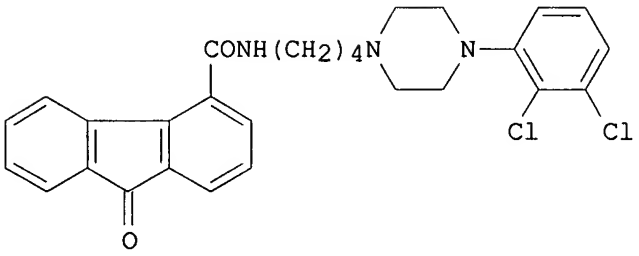
Relative stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:574757 CAPLUS
DOCUMENT NUMBER: 135:303847
TITLE: Design and Synthesis of [(2,3-Dichlorophenyl)piperazin-1-yl]alkylfluorenylcarboxamides as Novel Ligands Selective for the Dopamine D3 Receptor Subtype
AUTHOR(S): Robarge, Michael J.; Husbands, Stephen M.; Kieltyka, Andrzej; Brodbeck, Robbin; Thurkauf, Andrew; Newman, Amy Hauck
CORPORATE SOURCE: Medicinal Chemistry Section, National Institute on Drug Abuse-Intramural Research Program, Baltimore, MD, 21224, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(19), 3175-3186
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:303847
GI



I

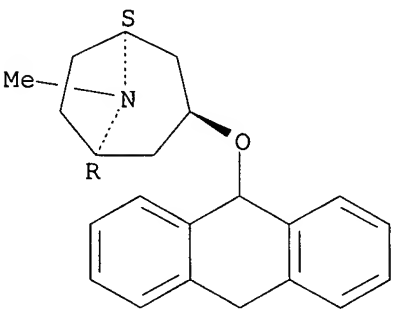
AB The dopamine D3 receptor subtype has been recently targeted as a potential neurochem. modulator of the behavioral actions of psychomotor stimulants, such as cocaine. However, definitive behavioral investigations have been hampered by the lack of highly selective D3 agonists and antagonists. In an attempt to design a novel class of D3 ligands with which to study this receptor system, a series of chemical divergent compds. that possessed various structural features that exist within several classes of reputed D3 agents was screened and compared to the recently reported NGB 2904. On the basis of these results, a novel series of compds. was designed that included functional moieties that were required for high-affinity and selective binding to D3 receptors. All the compds. in this series included an aryl-substituted piperazine ring, a varying alkyl chain linker (C3-C5), and a terminal aryl amide. The compds. were synthesized and evaluated in vitro for binding in CHO cells transfected with human D2, D3, or D4 receptor cDNAs. D3 binding affinities ranged from Ki = 1.4 to 1460 nM. The most potent analog in this series, I, demonstrated a D3/D2 selectivity of 64 and a D3/D4 selectivity of 1300. Structure-activity relationships for this class of ligands at D3 receptors will provide new leads toward the development of highly selective and potent mol. probes that will prove useful in the elucidation of the role D3 receptors play in the psychomotor stimulant and reinforcing properties of cocaine.

IT 367275-33-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of [(2,3-dichlorophenyl)piperazin-1-yl]alkylfluorenylcarboxamides as ligands selective for the dopamine D3 receptor)

RN 367275-33-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[(9,10-dihydro-9-anthracenyl)oxy]-8-methyl-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

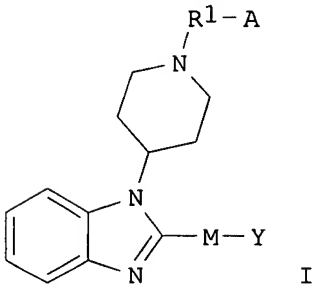


REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:573269 CAPLUS
DOCUMENT NUMBER: 135:152805
TITLE: Preparation of benzimidazoles as ORL1-receptor agonists for analgesics
INVENTOR(S): Ito, Fumitaka; Noguchi, Hirohide; Ohashi, Yoriko; Shimokawa, Hirohisa
PATENT ASSIGNEE(S): Pfizer Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
JP 2001213878	A	20010807	JP 2000-396414	20001227	<--
JP 3392402	B2	20030331			
EP 1122257	A1	20010808	EP 2000-311316	20001218	<--
EP 1122257	B1	20051012			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
AT 306488	T	20051015	AT 2000-311316	20001218	
ES 2249237	T3	20060401	ES 2000-311316	20001218	
CA 2330092	A1	20010705	CA 2001-2330092	20010103	<--
CA 2330092	C	20050322			
US 2002049212	A1	20020425	US 2001-753954	20010103	<--
US 6861425	B2	20050301			
BR 2001000014	A	20010828	BR 2001-14	20010104	<--
PRIORITY APPLN. INFO.:			US 2000-174542P P	20000105	

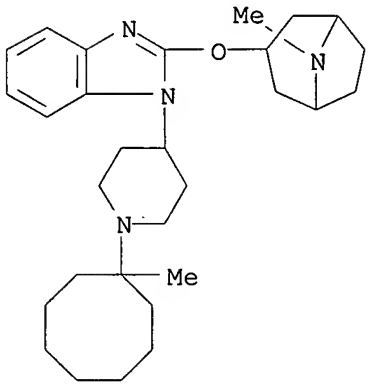
OTHER SOURCE(S): MARPAT 135:152805
GI



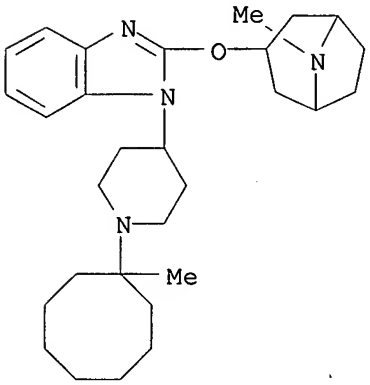
I

AB Title compds. I [R1 = C3-11 cycloalkyl, C6-16 bicycloalkyl, C6-16 tricycloalkyl, C8-16 tetracycloalkyl, etc.; A = (un)substituted C1-7 alkyl, C2-5 alkenyl, C2-5 alkynyl, aryl, etc.; M = single bond, CH2,O, S, SO, SO2, CO, NH, etc.; Y = 4- to 12-membered bicyclic carbon ring, 4- to 12- membered bicyclic hetero ring, 5- to 17-membered spiro carbon ring, 5- to 17-membered spiro hetero ring; Z1-Z4 = (un)substituted C1-4 alkyl, C1-4 alkoxy, C1-4 alkylsulfonyl, C1-4 alkylcarbonyl, carboxy, etc.] or their salts are prepared Tert-Bu 3-[1-[1-(1-phenylcycloheptyl)-4-piperidinyl]-1H-benzimidazol-2-yl]-3,8-diazabicyclo[3.2.1]octane-8-carboxylate was treated with F3CCO2H in CH2Cl2 at room temperature for 0.5 h to give 77.6% 2-(3,8-diazabicyclo[3.2.1]oct-3-yl)-1-[1-(1-phenylcycloheptyl)-4-piperidinyl]-1H-benzimidazole HCl salt.

IT 352542-54-2P 352542-55-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzimidazoles as ORL1-receptor agonists for analgesics)
RN 352542-54-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane, 8-methyl-3-[[1-[1-(1-methylcyclooctyl)-4-piperidinyl]-1H-benzimidazol-2-yl]oxy]- (9CI) (CA INDEX NAME)



RN 352542-55-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octane, 8-methyl-3-[[1-[1-(1-methylcyclooctyl)-4-piperidinyl]-1H-benzimidazol-2-yl]oxy]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L5 ANSWER 15 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:560443 CAPLUS
DOCUMENT NUMBER: 135:338915
TITLE: Optimization of a mathematical topological pattern for the prediction of antihistaminic activity
AUTHOR(S): Duart, M. J.; Garcia-Domenech, R.; Anton-Fos, G. M.; Galvez, J.
CORPORATE SOURCE: Departamento Ciencias Quimicas, Universidad Cardenal Herrera-CEU, Spain
SOURCE: Journal of Computer-Aided Molecular Design (2001), 15(6), 561-572
CODEN: JCADEQ; ISSN: 0920-654X
PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal
LANGUAGE: English

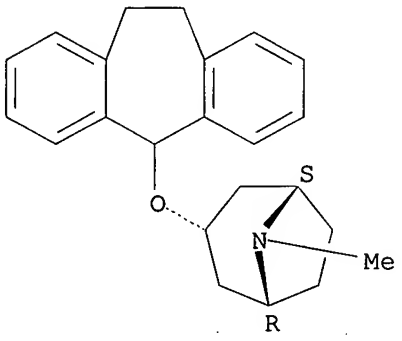
AB Mol. topol. was used to develop a math. model capable of classifying compds. according to antihistaminic activity. The equations used for this purpose were derived using multi-linear regression and linear discriminant anal. The topol. pattern of activity obtained allows the reliable prediction of antihistaminic activity in drugs frequently used for other therapeutic purposes. Based on the results, the proposed pattern is seemingly only valid for drugs that interact with histamine through competitive inhibition with H1 receptors.

IT 604-51-3, Deptropine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(optimization of a math. topol. pattern for the prediction of antihistaminic activity)

RN 604-51-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)oxy]-8-methyl-, (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:472716 CAPLUS
DOCUMENT NUMBER: 135:76801
TITLE: Preparation of 4-[aryl(8-azabicyclo[3.2.1]octan-3-yl)]aminobenzoic acid derivatives as delta-opioid receptor modulators
INVENTOR(S): Carson, John R.; Boyd, Robert E.; Neilson, Lou Anne
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046191	A1	20010628	WO 2000-US33055	20001204 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

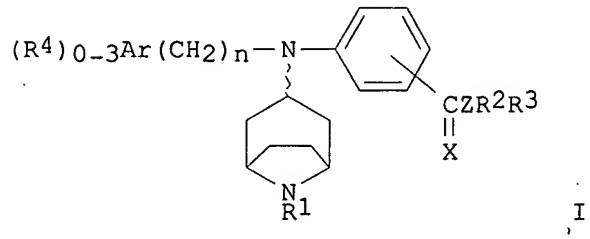
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2395471	A1	20010628	CA 2000-2395471		20001204 <--
US 6306876	B1	20011023	US 2000-728972		20001204 <--
EP 1242421	A1	20020925	EP 2000-983946		20001204 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2003518119	T	20030603	JP 2001-547101		20001204
PRIORITY APPLN. INFO.:			US 1999-171422P	P	19991222
			US 2000-728972	A	20001204
			WO 2000-US33055	W	20001204

OTHER SOURCE(S): MARPAT 135:76801

GI



I

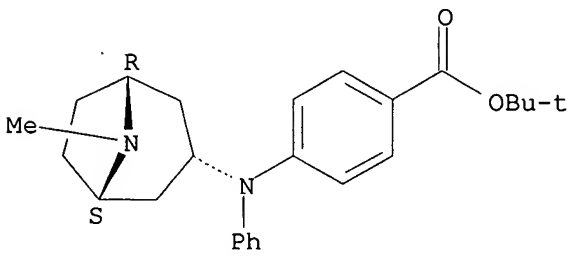
AB 4-[Aryl(8-azabicyclo[3.2.1]octan-3-yl)]aminobenzoic acid derivs. I [R1 = alkyl, alkenyl, cycloalkyl, etc.; R2, R3 = H, alkyl, = (un)substituted Ph, etc.; X = S, O; Z = N, O; n = 0, 1; Ar = Ph, 1-naphthyl, 2-naphthyl; R4 = OH, halo, alkyl, CF3, etc.], delta-opioid receptor modulators and useful as analgesics, were prepared E.g. a solution of 8-methyl-N-phenyl-endo-8-azabicyclo[3.2.1]octan-3-amine, N,N-diethyl-4-bromobenzamide, tris(dibenzylideneacetone)dipalladium(0), tri-tert-butylphosphine, and sodium tert-butoxide in dry toluene was heated at about 110°C under argon in a pressure vessel for about 16 h. to give N,N-diethyl-4-[phenyl(endo-8-methyl-8-azabicyclo[3.2.1]octan-3-yl)amino]benzamide isolated as 1:1 fumarate salt.

IT 287721-06-6P 287721-10-2P 346708-36-9P
346708-40-5P 346708-46-1P 346708-47-2P
347888-67-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 4-[aryl(8-azabicyclo[3.2.1]octan-3-yl)]aminobenzoic acid derivs. as delta-opioid receptor modulators)

RN 287721-06-6 CAPLUS

CN Benzoic acid, 4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

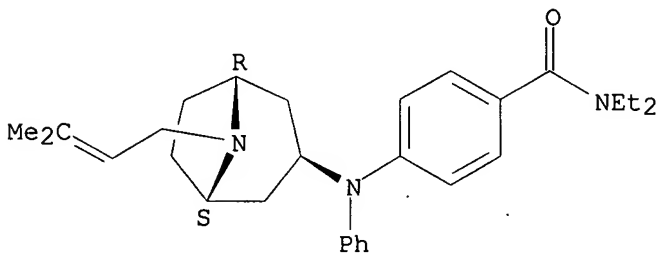
Relative stereochemistry.



RN 287721-10-2 CAPLUS

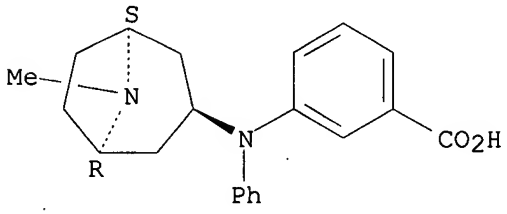
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-(3-methyl-2-butenyl)-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 346708-36-9 CAPLUS
CN Benzoic acid, 3-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, dihydrochloride (9CI) (CA INDEX NAME)

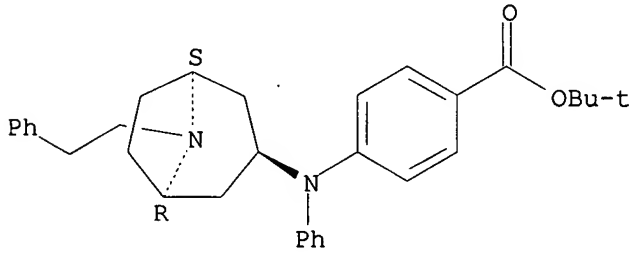
Relative stereochemistry.



●2 HCl

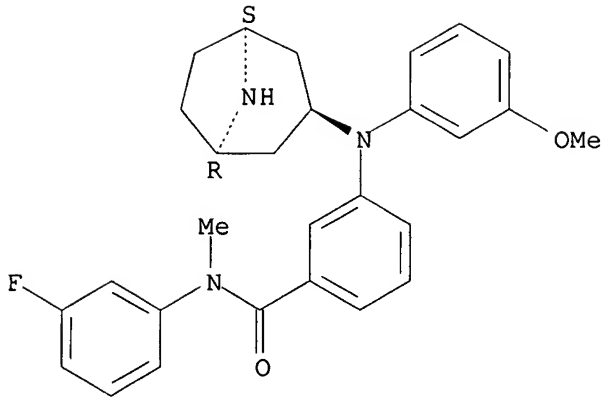
RN 346708-40-5 CAPLUS
CN Benzoic acid, 4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



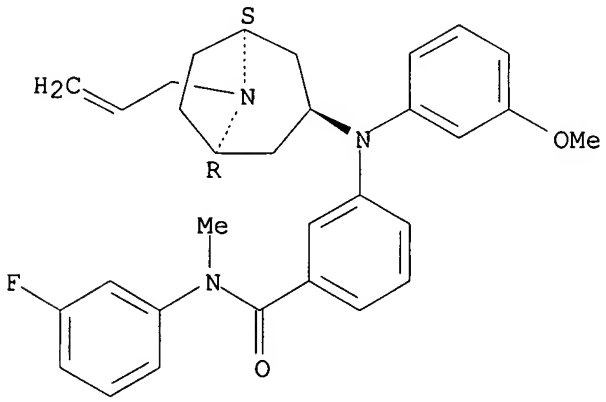
RN 346708-46-1 CAPLUS
CN Benzamide, 3-[(3-endo)-8-azabicyclo[3.2.1]oct-3-yl(3-methoxyphenyl)amino]-N-(3-fluorophenyl)-N-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



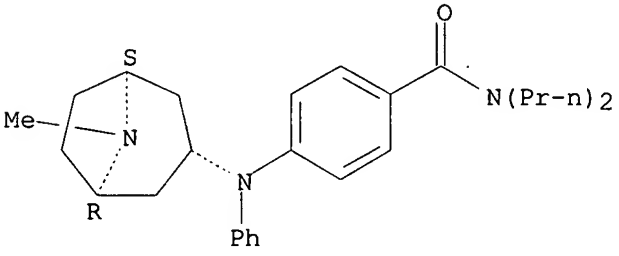
RN 346708-47-2 CAPLUS
CN Benzamide, N-(3-fluorophenyl)-3-[(3-methoxyphenyl)[(3-endo)-8-(2-propenyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-N-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 347888-67-9 CAPLUS
CN Benzamide, 4-[[(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N,N-dipropyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

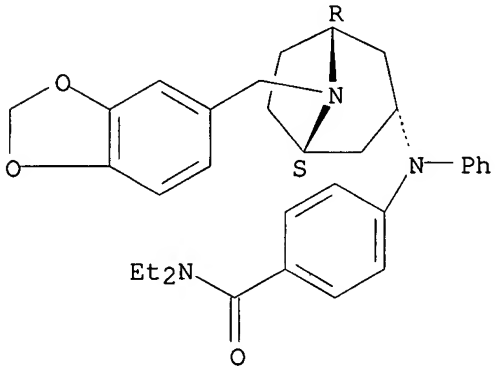


IT 287720-74-5P 287720-78-9P 287720-81-4P
287720-83-6P 287720-85-8P 287720-86-9P
287720-88-1P 287720-90-5P 287720-94-9P
287720-96-1P 287720-97-2P 287720-98-3P
287721-03-3P 287721-07-7P 287721-08-8P
287721-09-9P 287721-11-3P 287721-13-5P
287721-15-7P 287721-16-8P 287729-25-3P
287729-26-4P 287729-27-5P 287729-28-6P
287729-29-7P 346708-06-3P 346708-07-4P

346708-08-5P 346708-10-9P 346708-11-0P
346708-12-1P 346708-13-2P 346708-14-3P
346708-16-5P 346708-17-6P 346708-24-5P
346708-26-7P 346708-28-9P 346708-29-0P
346708-34-7P 346708-38-1P 346708-41-6P
346708-42-7P 346708-43-8P 346708-45-0P
346708-49-4P 347888-66-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-[aryl(8-azabicyclo[3.2.1]octan-3-yl)]aminobenzoic acid derivs. as delta-opioid receptor modulators)

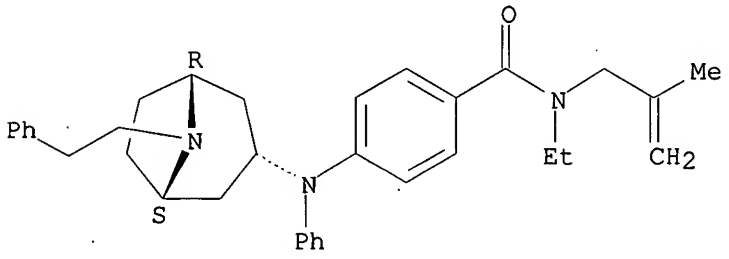
RN 287720-74-5 CAPLUS
CN Benzamide, 4-[[(3-endo)-8-(1,3-benzodioxol-5-ylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N,N-diethyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



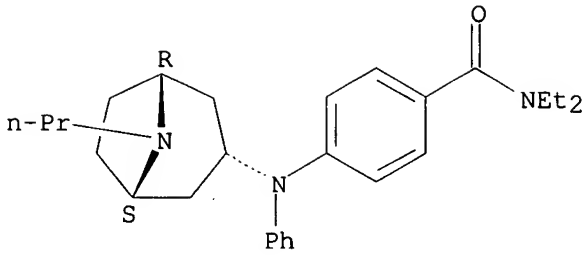
RN 287720-78-9 CAPLUS
CN Benzamide, N-ethyl-N-(2-methyl-2-propenyl)-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



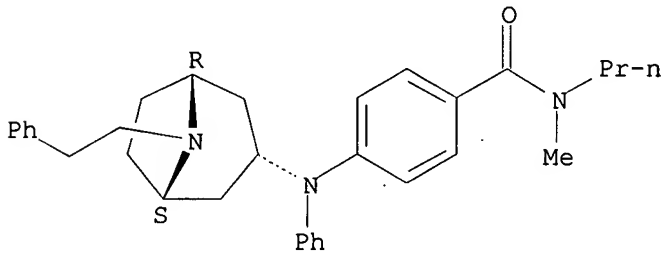
RN 287720-81-4 CAPLUS
CN Benzamide, N,N-diethyl-4-[phenyl[(3-endo)-8-propyl-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



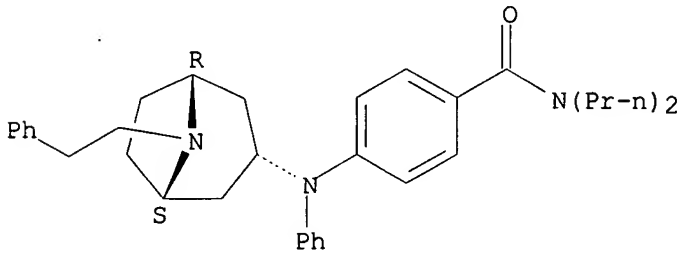
RN 287720-83-6 CAPLUS
CN Benzamide, N-methyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-N-propyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



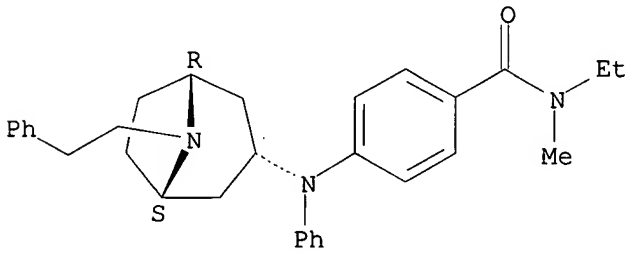
RN 287720-85-8 CAPLUS
CN Benzamide, 4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-N,N-dipropyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 287720-86-9 CAPLUS
CN Benzamide, N-ethyl-N-methyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

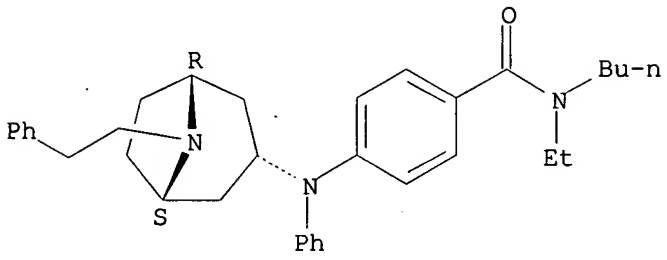
Relative stereochemistry.



RN 287720-88-1 CAPLUS
CN Benzamide, N-butyl-N-ethyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-

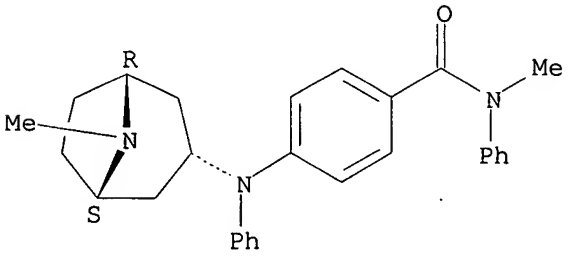
azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



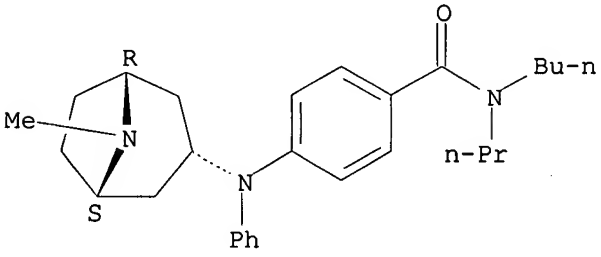
RN 287720-90-5 CAPLUS
CN Benzamide, N-methyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



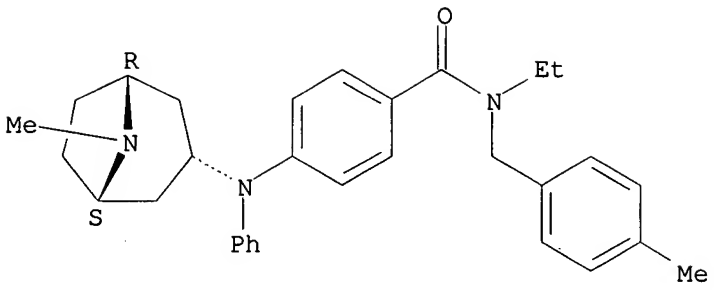
RN 287720-94-9 CAPLUS
CN Benzamide, N-butyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N-propyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



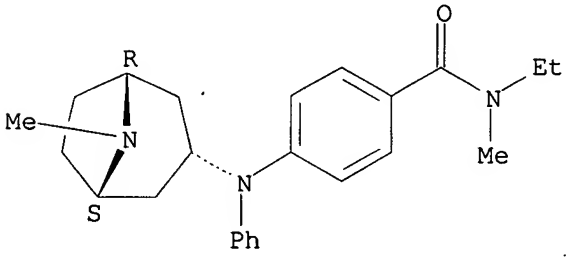
RN 287720-96-1 CAPLUS
CN Benzamide, N-ethyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



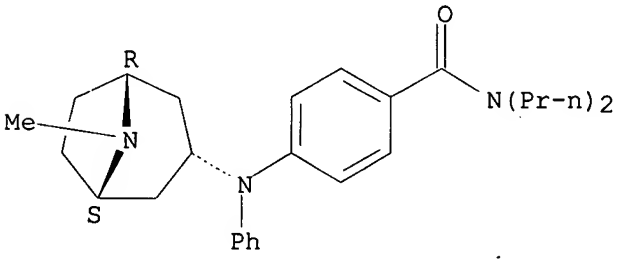
RN 287720-97-2 CAPLUS
CN Benzamide, N-ethyl-N-methyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



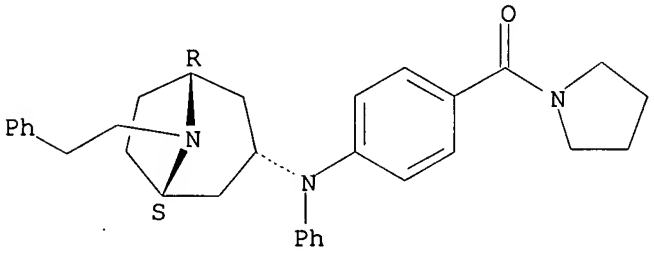
RN 287720-98-3 CAPLUS
CN Benzamide, 4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N,N-dipropyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 287721-03-3 CAPLUS
CN Pyrrolidine, 1-[4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]benzoyl]- (9CI) (CA INDEX NAME)

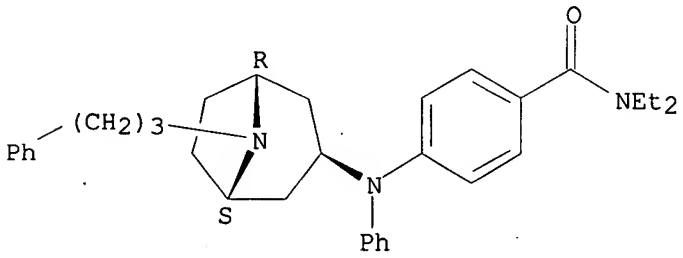
Relative stereochemistry.



RN 287721-07-7 CAPLUS

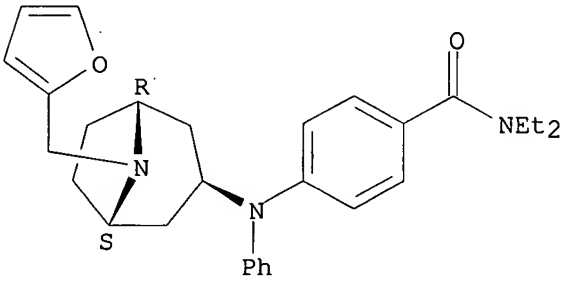
CN Benzamide, N,N-diethyl-4-[phenyl[(3-exo)-8-(3-phenylpropyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



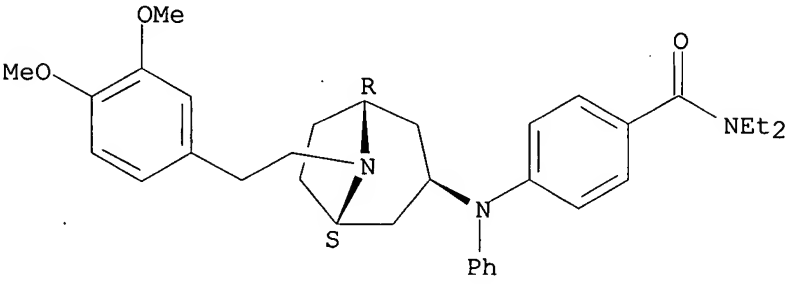
RN 287721-08-8 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-(2-furanylmethyl)-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



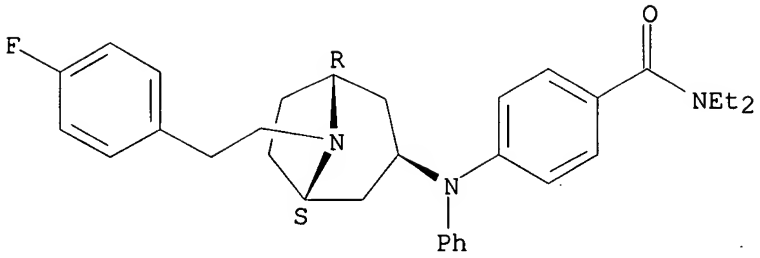
RN 287721-09-9 CAPLUS
CN Benzamide, 4-[[(3-exo)-8-[2-(3,4-dimethoxyphenyl)ethyl]-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N,N-diethyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



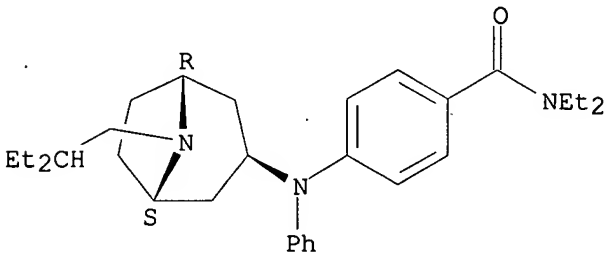
RN 287721-11-3 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-[2-(4-fluorophenyl)ethyl]-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



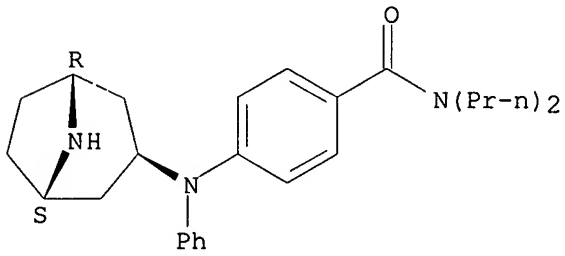
RN 287721-13-5 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-(2-ethylbutyl)-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



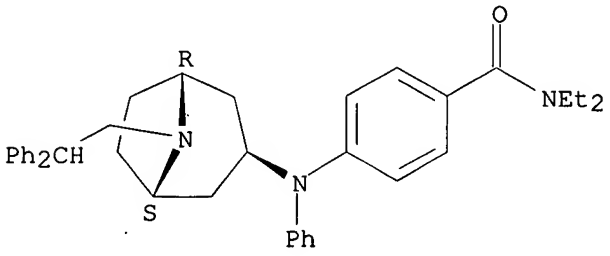
RN 287721-15-7 CAPLUS
CN Benzamide, 4-[(3-exo)-8-azabicyclo[3.2.1]oct-3-ylphenylamino]-N,N-dipropyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 287721-16-8 CAPLUS
CN Benzamide, 4-[[(3-exo)-8-(2,2-diphenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N,N-diethyl- (9CI) (CA INDEX NAME)

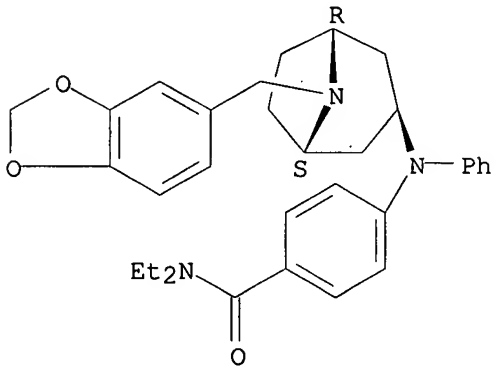
Relative stereochemistry.



RN 287729-25-3 CAPLUS
CN Benzamide, 4-[[(3-exo)-8-(1,3-benzodioxol-5-ylmethyl)-8-

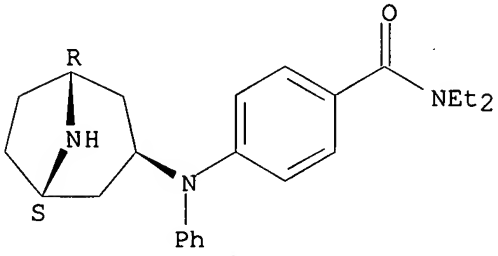
azabicyclo[3.2.1]oct-3-yl]phenylamino]-N,N-diethyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



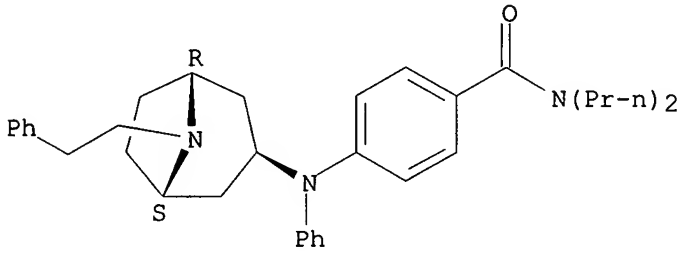
RN 287729-26-4 CAPLUS
CN Benzamide, 4-[(3-exo)-8-azabicyclo[3.2.1]oct-3-ylphenylamino]-N,N-diethyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



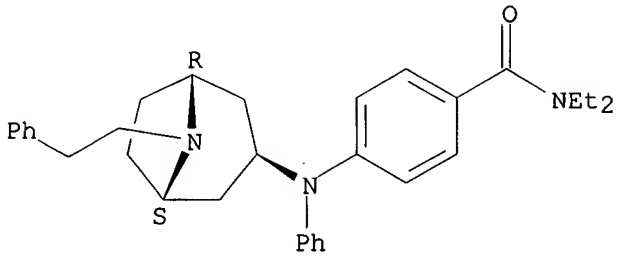
RN 287729-27-5 CAPLUS
CN Benzamide, 4-[phenyl[(3-exo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-N,N-dipropyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



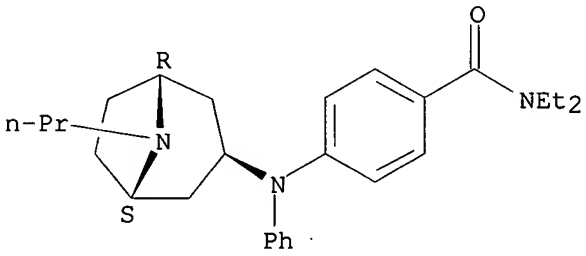
RN 287729-28-6 CAPLUS
CN Benzamide, N,N-diethyl-4-[phenyl[(3-exo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 287729-29-7 CAPLUS
CN Benzamide, N,N-diethyl-4-[phenyl[(3-exo)-8-propyl-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

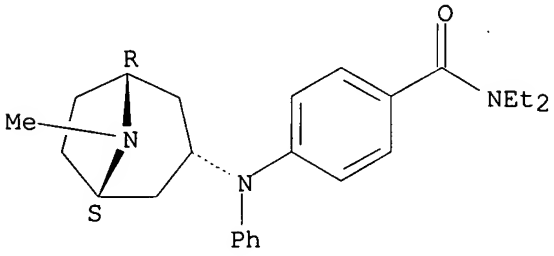


RN 346708-06-3 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 287720-73-4
CMF C25 H33 N3 O

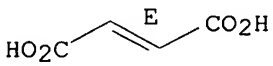
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



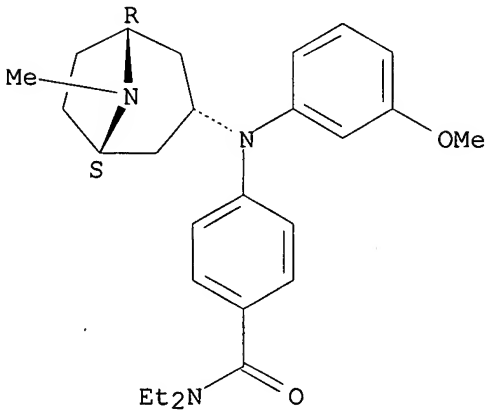
RN 346708-07-4 CAPLUS
CN Benzamide, N,N-diethyl-4-[(3-methoxyphenyl)[(3-endo)-8-methyl-8-

azabicyclo[3.2.1]oct-3-yl]amino]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 287720-99-4
CMF C26 H35 N3 O2

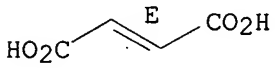
Relative stereochemistry.



CM 2

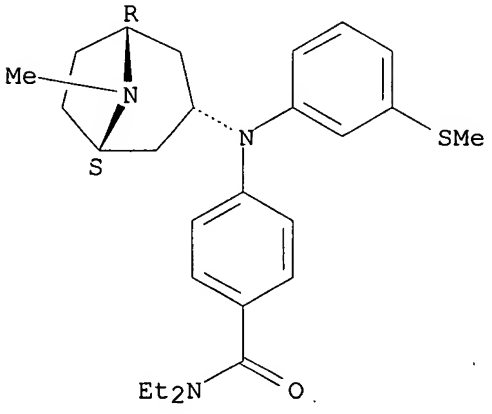
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 346708-08-5 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl][3-(methylthio)phenyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



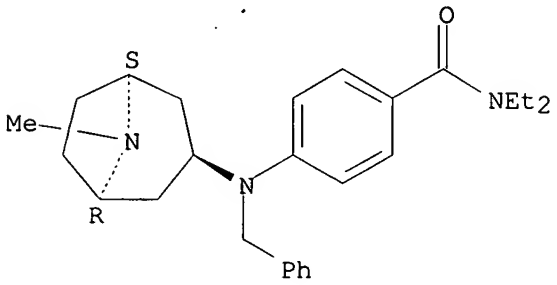
● HCl

RN 346708-10-9 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl](phenylmethyl)amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

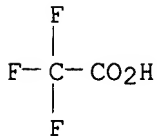
CRN 346708-09-6
CMF C26 H35 N3 O

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

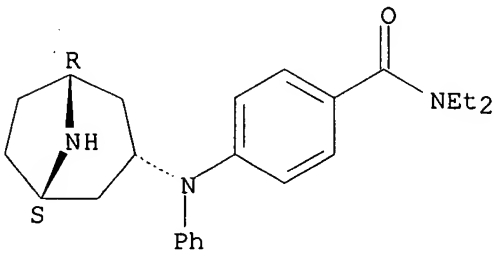


RN 346708-11-0 CAPLUS
CN Benzamide, 4-[(3-endo)-8-azabicyclo[3.2.1]oct-3-ylphenylamino]-N,N-diethyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 287720-75-6
CMF C24 H31 N3 O

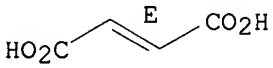
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

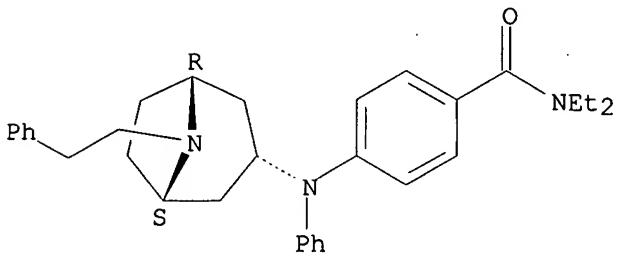


RN 346708-12-1 CAPLUS
CN Benzamide, N,N-diethyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 287720-92-7
CMF C32 H39 N3 O

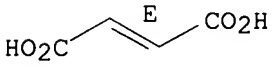
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

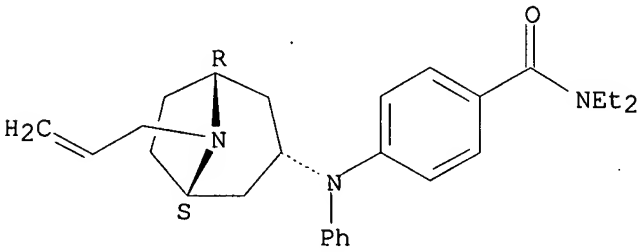


RN 346708-13-2 CAPLUS
CN Benzamide, N,N-diethyl-4-[phenyl[(3-endo)-8-(2-propenyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

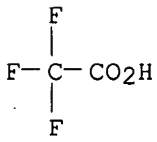
CRN 287720-76-7
CMF C27 H35 N3 O

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

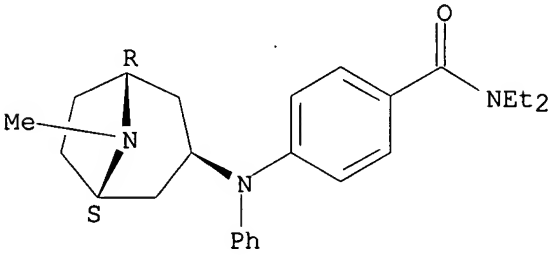


RN 346708-14-3 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 287729-31-1
CMF C25 H33 N3 O

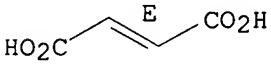
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

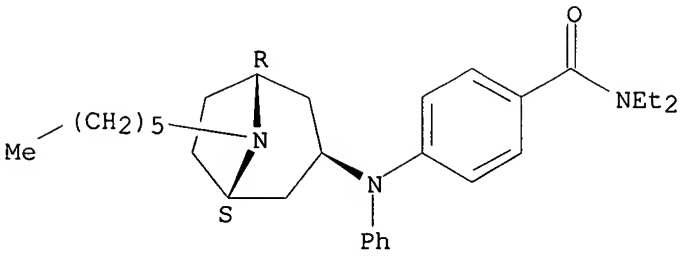


RN 346708-16-5 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-hexyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 287721-12-4
CMF C30 H43 N3 O

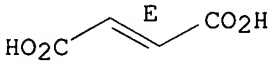
Relative stereochemistry.



CM 2

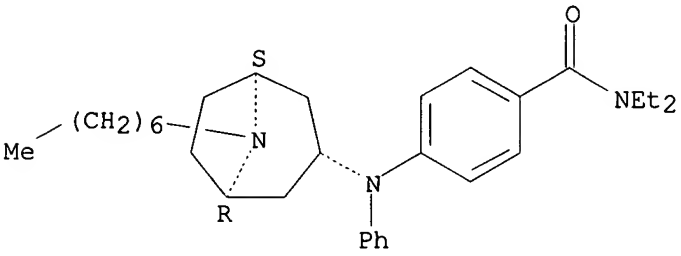
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 346708-17-6 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-heptyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

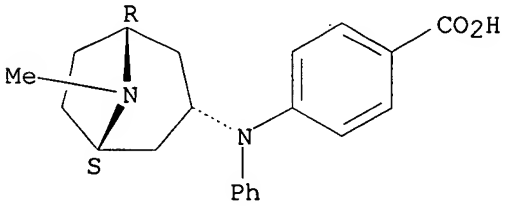


RN 346708-24-5 CAPLUS
CN Benzoic acid, 4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 287721-05-5
CMF C21 H24 N2 O2

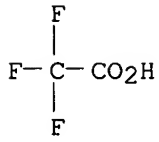
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2

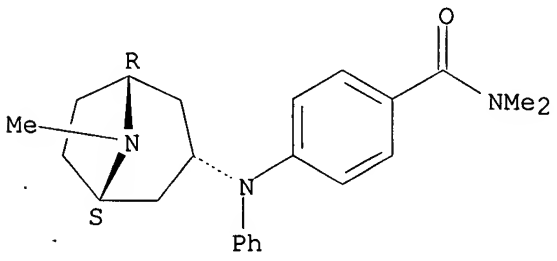


RN 346708-26-7 CAPLUS
CN Benzamide, N,N-dimethyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

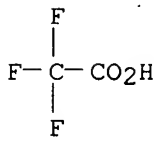
CRN 287721-02-2
CMF C23 H29 N3 O

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

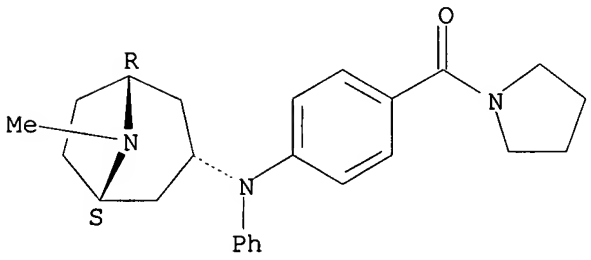


RN 346708-28-9 CAPLUS
CN Pyrrolidine, 1-[4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]benzoyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

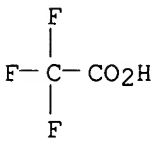
CRN 287721-01-1
CMF C25 H31 N3 O

Relative stereochemistry.



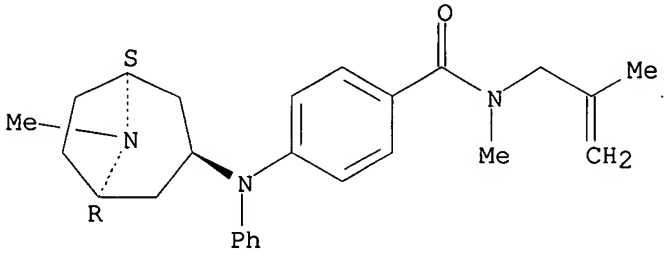
CM 2

CRN 76-05-1
CMF C2 H F3 O2



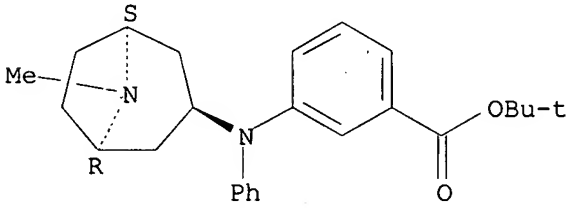
RN 346708-29-0 CAPLUS
CN Benzamide, N-methyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-N-(2-methyl-2-propenyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 346708-34-7 CAPLUS
CN Benzoic acid, 3-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



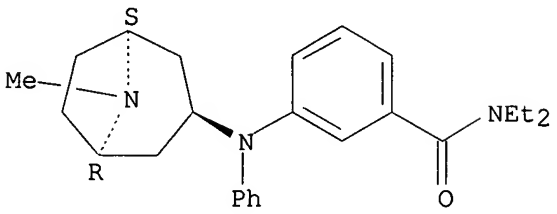
RN 346708-38-1 CAPLUS
CN Benzamide, N,N-diethyl-3-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 346708-37-0

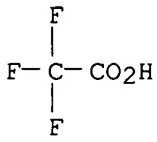
CMF C25 H33 N3 O

Relative stereochemistry.



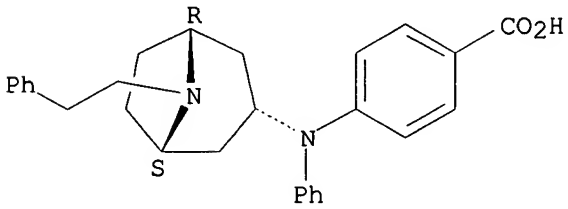
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 346708-41-6 CAPLUS
CN Benzoic acid, 4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



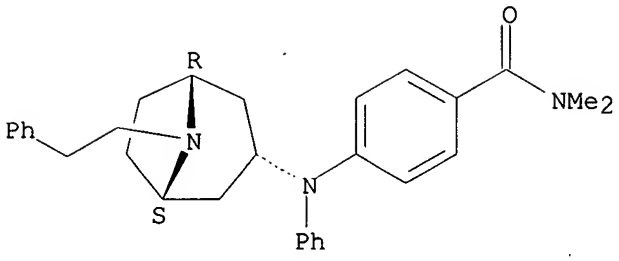
● HCl

RN 346708-42-7 CAPLUS
CN Benzamide, N,N-dimethyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 287721-00-0
CMF C30 H35 N3 O

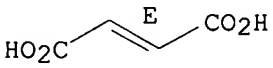
Relative stereochemistry.



CM 2

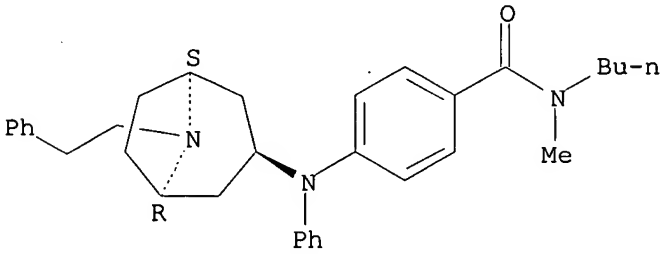
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 346708-43-8 CAPLUS
CN Benzamide, N-butyl-N-methyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

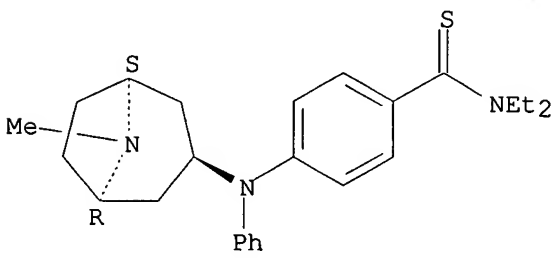


RN 346708-45-0 CAPLUS
CN Benzenecarbothioamide, N,N-diethyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

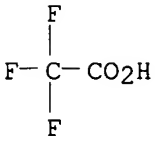
CRN 346708-44-9
CMF C25 H33 N3 S

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

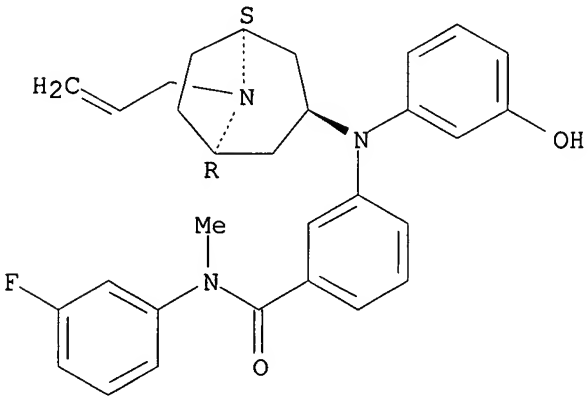


RN 346708-49-4 CAPLUS
CN Benzamide, N-(3-fluorophenyl)-3-[(3-hydroxyphenyl)[(3-endo)-8-(2-propenyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]-N-methyl-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

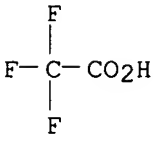
CRN 346708-48-3
CMF C30 H32 F N3 O2

Relative stereochemistry.



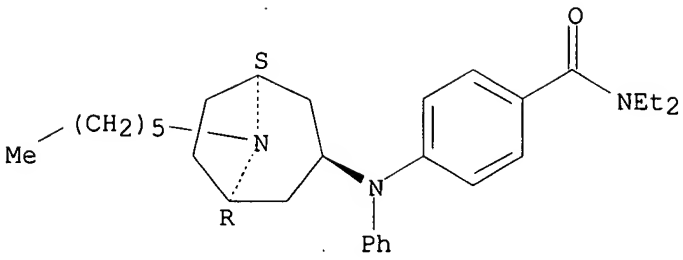
CM 2

CRN 76-05-1
CMF C2 H F3 O2



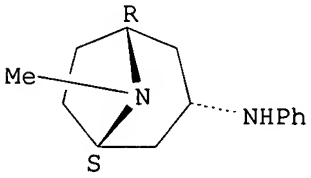
RN 347888-66-8 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-endo)-8-hexyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



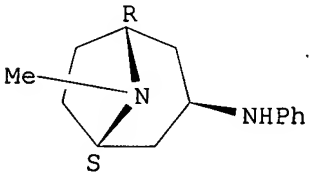
IT 63930-13-2 63930-14-3 346708-51-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-[aryl(8-azabicyclo[3.2.1]octan-3-yl)]aminobenzoic acid derivs. as delta-opioid receptor modulators)
RN 63930-13-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-methyl-N-phenyl-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



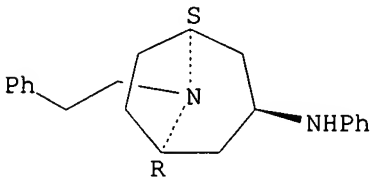
RN 63930-14-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-methyl-N-phenyl-, (3-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 346708-51-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-phenyl-8-(2-phenylethyl)-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



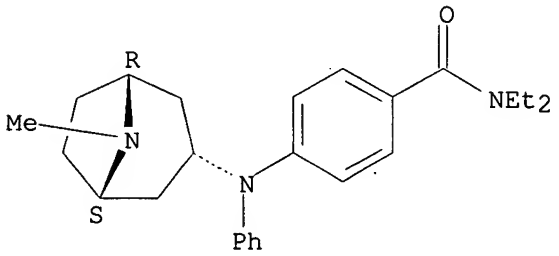
IT 287720-73-4P 287720-75-6P 287720-92-7P
287721-00-0P 287721-05-5P 287729-31-1P
289468-30-0P 346708-53-0P 346708-54-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4-[aryl(8-azabicyclo[3.2.1]octan-3-yl)]aminobenzoic acid

derivs. as delta-opioid receptor modulators)

RN 287720-73-4 CAPLUS

CN Benzamide, N,N-diethyl-4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

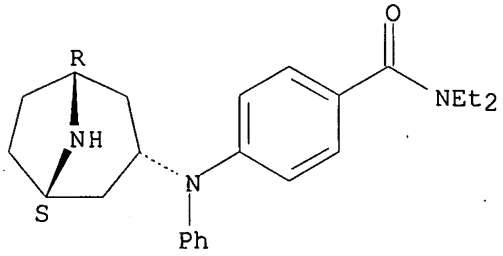
Relative stereochemistry.



RN 287720-75-6 CAPLUS

CN Benzamide, 4-[(3-endo)-8-azabicyclo[3.2.1]oct-3-ylphenylamino]-N,N-diethyl- (9CI) (CA INDEX NAME)

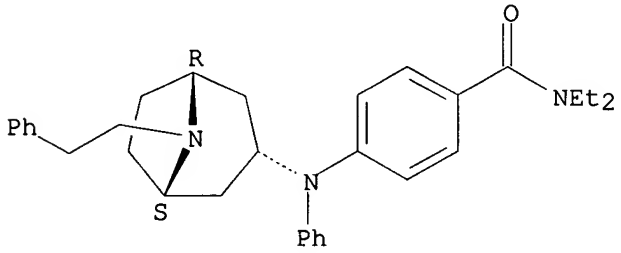
Relative stereochemistry.



RN 287720-92-7 CAPLUS

CN Benzamide, N,N-diethyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

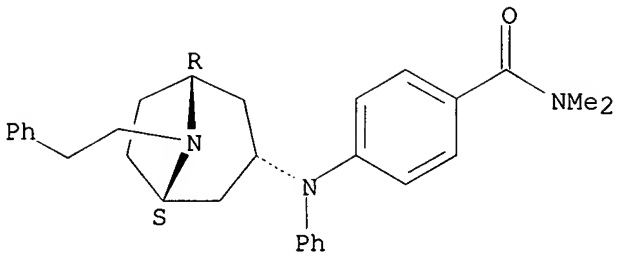
Relative stereochemistry.



RN 287721-00-0 CAPLUS

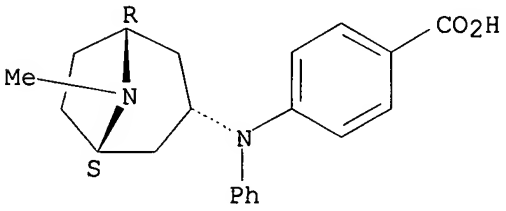
CN Benzamide, N,N-dimethyl-4-[phenyl[(3-endo)-8-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-3-yl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



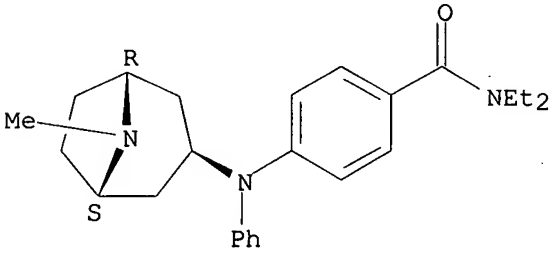
RN 287721-05-5 CAPLUS
CN Benzoic acid, 4-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



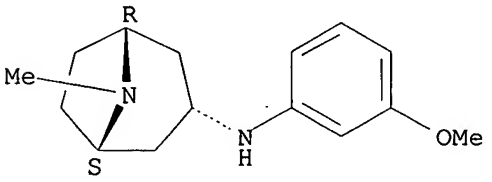
RN 287729-31-1 CAPLUS
CN Benzamide, N,N-diethyl-4-[[(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



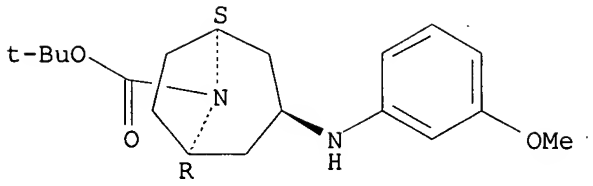
RN 289468-30-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octan-3-amine, N-(3-methoxyphenyl)-8-methyl-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



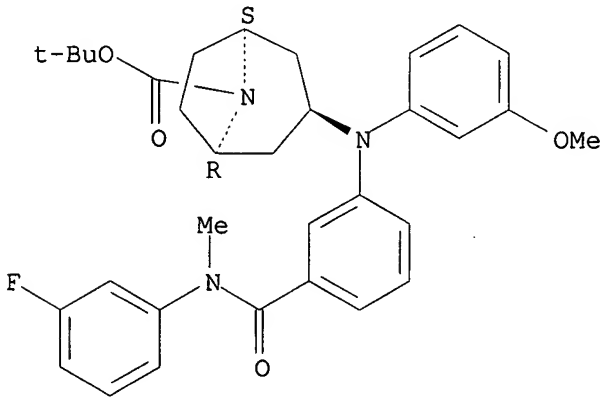
RN 346708-53-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-carboxylic acid, 3-[(3-methoxyphenyl)amino]-, 1,1-dimethylethyl ester, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 346708-54-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-carboxylic acid, 3-[[3-[[(3-fluorophenyl)methylamino]carbonyl]phenyl](3-methoxyphenyl)amino]-, 1,1-dimethylethyl ester, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:380340 CAPLUS
DOCUMENT NUMBER: 135:9993
TITLE: Transdermal delivery system for alkaloids of Aconitum species
INVENTOR(S): Xiong, Weihong; Patel, Dinesh C.
PATENT ASSIGNEE(S): Xel Herbaceuticals, USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001035883	A1	20010525	WO 2000-US31821	20001117 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-166497P P 19991119
US 2000-249380P P 20001116

AB The present invention provides a composition of transdermally administered aconitine alkaloids for ameliorating pain and inflammation. In one

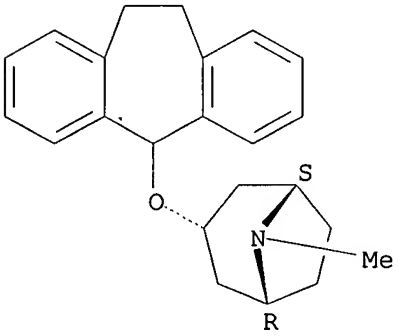
aspect, an aconitine alkaloid is delivered in a sufficient amount to achieve and maintain a blood plasma aconitine alkaloid level of about 0.5 ng/mL to about 400 ng/mL. Aconitine alkaloids may be delivered by themselves, or in combination with other elements, such as addnl. analgesics, other drugs, or pos. health promoting substances. Various formulations for the transdermal delivery of aconitine alkaloids are disclosed, and may include selected penetration enhancers. Thus, a cream contained aconitine 0.01-40, stearic acid 0.1-30, stearyl alc. 0.1-10, cetyl alc. 0.1-10, glycerin 1-30, methylparaben 0.01-2, propylparaben 0.01-2, KOH 0.01-3, and water 40-95%.

IT 604-51-3, Deptropine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(transdermal delivery system for alkaloids of Aconitum species)

RN 604-51-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)oxy]-8-methyl-, (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:841966 CAPLUS

DOCUMENT NUMBER: 134:13350

TITLE: Nitric oxide synthase (NOS) inhibitor combinations with other agents for treatment of disorders treatable by altering circadian rhythm

INVENTOR(S): Saltarelli, Mario David; Lowe, John Adams, III

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 113 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000071107	A2	20001130	WO 2000-IB295	20000316 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2374668	A1	20001130	CA 2000-2374668	20000316 <--
EP 1178784	A1	20020213	EP 2000-907891	20000316 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO

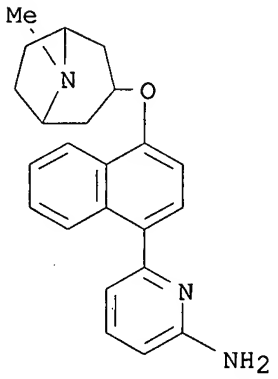
BR 2000010820	A	20020305	BR 2000-10820		20000316 <--
TR 200103351	T2	20020621	TR 2001-3351		20000316 <--
EE 200100611	A	20030217	EE 2001-611		20000316
JP 2003523941	T	20030812	JP 2000-619414		20000316
HU 200301287	A2	20030828	HU 2003-1287		20000316
HU 200301287	A3	20050329			
CN 1617743	A	20050518	CN 2000-807878		20000316
IN 2000MU00445	A	20050304	IN 2000-MU445		20000515
NO 2001005651	A	20020118	NO 2001-5651		20011120 <--
HR 2001000862	A1	20030630	HR 2001-862		20011120
ZA 2001009555	A	20040407	ZA 2001-9555		20011120
BG 106208	A	20020930	BG 2001-106208		20011211 <--
PRIORITY APPLN. INFO.:			US 1999-135520P	P	19990521
			WO 2000-IB295	W	20000316

AB New pharmaceutical uses are provided for compds. that exhibit activity as NOS inhibitors. Specifically, the invention provides the use of NOS inhibitors, particularly selective neuronal NOS (nNOS) inhibitors, alone or in combination with another active agent, in particular, either a selective serotonin reuptake inhibitor (SSRI) or an NK-1 receptor antagonist, for the treatment of disorders or conditions the treatment which can be effected or facilitated by altering circadian rhythms. Examples of such disorders and conditions are blindness, obesity, seasonal affective disorder, bipolar disorder, jet lag, circadian sleep rhythms disorder, sleep deprivation, parasomnias, REM sleep disorders, hypersomnia, sleep-wake cycle disorders, narcolepsy and sleep disorders associated with shift work or irregular work schedules; nocturnal enuresis, and restless-legs syndrome.

IT 310431-78-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nitric oxide synthase inhibitor combinations with other agents for treatment of disorders treatable by altering circadian rhythm)

RN 310431-78-8 CAPLUS

CN 2-Pyridinamine, 6-[4-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)oxy]-1-naphthalenyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 19 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN

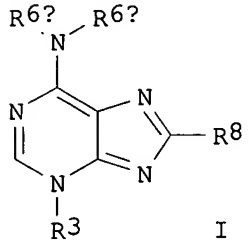
ACCESSION NUMBER:	2000:725418 CAPLUS
DOCUMENT NUMBER:	133:296324
TITLE:	Synthesis and phosphodiesterase IV inhibition activity of purine derivatives
INVENTOR(S):	Chasin, Mark; Cavalla, David; Hofer, Peter; Gehrig, Andre; Wintergest, Peter
PATENT ASSIGNEE(S):	Euro-Celtique S.A., Luxembourg
SOURCE:	PCT Int. Appl., 112 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

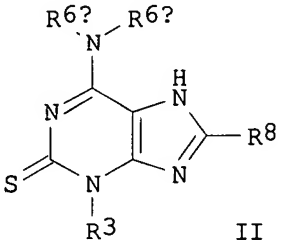
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059449	A2	20001012	WO 2000-US8525	20000331 <--
WO 2000059449	A3	20010104		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
CA 2367143	A1	20001012	CA 2000-2367143	20000331 <--
EP 1169321	A2	20020109	EP 2000-919929	20000331 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
HU 200200938	A2	20021028	HU 2002-938	20000331 <--
JP 2002541078	T	20021203	JP 2000-609014	20000331 <--
BR 2000011182	A	20030610	BR 2000-11182	20000331
JP 2001316314	A	20011113	JP 2000-136383	20000509 <--

PRIORITY APPLN. INFO.:	US 1999-285473	A	19990402
	IN 1994-CA514	A1	19940630
	WO 2000-US8525	W	20000331

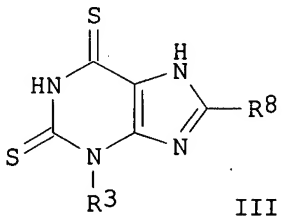
OTHER SOURCE(S): MARPAT 133:296324
GI



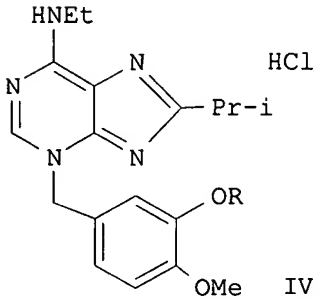
I



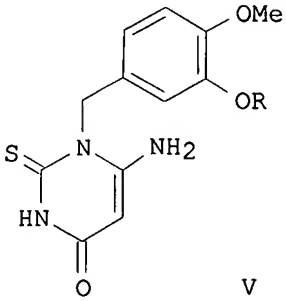
II



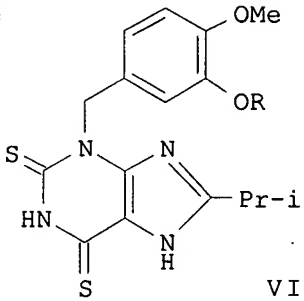
III



IV



V



VI

AB The purine (I) (R3, R8, R6a, R6b = H, (un)substituted alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, heteroaryl etc.), thioisoguanine (II), dithioxanthine (III) derivs., and their pharmaceutically accepted salts were synthesized. Thus, purine (IV; R = (CH2)5) was prepared by

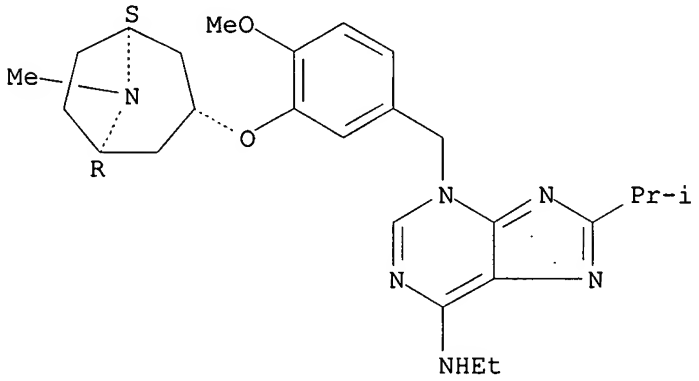
etherification of isovanilline with cyclopentanol, oximation, reduction to amine, conversion to isothiocyanate, amination to thiourea followed by heterocyclization with Et cyanoacetate to thiouracil (V). V was nitrosylated, reduced, reacted with isobutyric anhydride to give isobutyrylamine which on treatment with phosphorus pentasulfide gave dithioxanthine (VI). VI, in a pressure reactor gave purine-2-thione which was reduced with Raney-nickel to give IV. The IC50 of IV against phosphodiesterase IV inhibition was 0.32 μM. I, II and III were effective in effecting PDE IV inhibition in patients in need thereof.

IT 300784-31-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purine derivs. as phosphodiesterase IV inhibitors)

RN 300784-31-0 CAPLUS

CN 3H-Purin-6-amine, N-ethyl-3-[[4-methoxy-3-[[(3-exo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]oxy]phenyl]methyl]-8-(1-methylethyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 20 OF 189 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:720700 CAPLUS

DOCUMENT NUMBER: 134:25113

TITLE: Classification of multidrug-resistance reversal agents using structure-based descriptors and linear discriminant analysis

AUTHOR(S): Bakken, Gregory A.; Jurs, Peter C.

CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Journal of Medicinal Chemistry (2000), 43(23), 4534-4541
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Linear discriminant anal. is used to generate models to classify multidrug-resistance reversal agents based on activity. Models are generated and evaluated using multidrug-resistance reversal activity values for 609 compds. measured using adriamycin-resistant P388 murine leukemia cells. Structure-based descriptors numerically encode mol. features which are used in model formation. Two types of models are generated: one type to classify compds. as inactive, moderately active, and active (three-class problem) and one type to classify compds. as inactive or active without considering the moderately active class (two-class problem). Two activity distributions are considered, where the separation between inactive and active compds. is different. When the separation between inactive and active classes is small, a model based on nine topol.

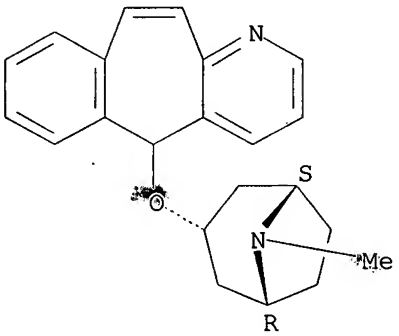
descriptors is developed that produces a classification rate of 83.1% correct for an external prediction set. Larger separation between active and inactive classes raises the prediction set classification rate to 92.0% correct using a model with six topol. descriptors. Models are further validated through Monte Carlo expts. in which models are generated after class labels have been scrambled. The classification rates achieved demonstrate that the models developed could serve as a screening mechanism to identify potentially useful multidrug-resistance reversal (MDRR) agents from large libraries of compds.

IT 19410-02-7, Tropirine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(classification of multidrug-resistance reversal agents using structure-based descriptors and linear discriminant anal. in relation to drug screening)

RN 19410-02-7 CAPLUS

CN 5H-Benzo[4,5]cyclohepta[1,2-b]pyridine, 5-[[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]oxy]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 10:22:30 ON 15 MAY 2007)

FILE 'REGISTRY' ENTERED AT 10:22:39 ON 15 MAY 2007
L1 STRUCTURE UPLOADED
L2 50 S L1
L3 1572 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:23:34 ON 15 MAY 2007
L4 270 S L3 FULL
L5 189 S L4 AND PY<2003

FILE 'STNGUIDE' ENTERED AT 10:28:59 ON 15 MAY 2007

FILE 'CAPLUS' ENTERED AT 10:32:36 ON 15 MAY 2007

FILE 'STNGUIDE' ENTERED AT 10:32:44 ON 15 MAY 2007

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.18	285.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-15.60

STN INTERNATIONAL LOGOFF AT 10:34:35 ON 15 MAY 2007